

FORM PTO-1390 (REV. 11-2000)		U.S. DEPARTMENT OF COMMERCE PATENT AND TRADEMARK OFFICE		ATTORNEY'S DOCKET NUMBER 54203-H-PCT-US/JPW/SHS	
TRANSMITTAL LETTER TO THE UNITED STATES DESIGNATED/ELECTED OFFICE (DO/EO/US) CONCERNING A FILING UNDER 35 U.S.C. 371				U.S. APPLICATION NO. (If known, see 37 CFR 1.5 Not Yet Known <b>09/856200</b>	
INTERNATIONAL APPLICATION NO. PCT/US98/23905		INTERNATIONAL FILING DATE 10 November 1998		PRIORITY DATE CLAIMED 10 November 1997	
TITLE OF INVENTION CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN gp120					
APPLICANT(S) FOR DO/EO/US Peter D. Kwong et al.					
Applicant herewith submits to the United States Designated/Elected Office (DO/EO/US) the following items and other information:					
1. <input checked="" type="checkbox"/> This is a <b>FIRST</b> submission of items concerning a filing under 35 U.S.C. 371. 2. <input type="checkbox"/> This is a <b>SECOND</b> or <b>SUBSEQUENT</b> submission of items concerning a filing under 35 U.S.C. 371. 3. <input type="checkbox"/> This is an express request to begin national examination procedures (35 U.S.C. 371(f)). The submission must include items (5), (6), (9) and (21) indicated below. 4. <input checked="" type="checkbox"/> The US has been elected by the expiration of 19 months from the priority date (Article 31). 5. <input checked="" type="checkbox"/> A copy of the International Application as filed (35 U.S.C. 371(c)(2)) a. <input type="checkbox"/> is attached hereto (required only if not communicated by the International Bureau). b. <input type="checkbox"/> has been communicated by the International Bureau. c. <input checked="" type="checkbox"/> is not required, as the application was filed in the United States Receiving Office (RO/US). 6. <input type="checkbox"/> An English language translation of the International Application as filed (35 U.S.C. 371(c)(2)). a. <input type="checkbox"/> is attached hereto. b. <input type="checkbox"/> has been previously submitted under 35 U.S.C. 154(d)(4). 7. <input checked="" type="checkbox"/> Amendments to the claims of the International Application under PCT Article 19 (35 U.S.C. 371(c)(3)) a. <input type="checkbox"/> are attached hereto (required only if not communicated by the International Bureau). b. <input type="checkbox"/> have been communicated by the International Bureau. c. <input type="checkbox"/> have not been made; however, the time limit for making such amendments has NOT expired. d. <input checked="" type="checkbox"/> have not been made and will not be made. 8. <input type="checkbox"/> An English language translation of the amendments to the claims under PCT Article 19 (35 U.S.C. 371 (c)(3)). 9. <input type="checkbox"/> An oath or declaration of the inventor(s) (35 U.S.C. 371(c)(4)). 10. <input type="checkbox"/> An English language translation of the annexes of the International Preliminary Examination Report under PCT Article 36 (35 U.S.C. 371(c)(5)).					
<b>Items 11 to 20 below concern document(s) or information included:</b>					
11. <input type="checkbox"/> An Information Disclosure Statement under 37 CFR 1.97 and 1.98. 12. <input type="checkbox"/> An assignment document for recording. A separate cover sheet in compliance with 37 CFR 3.28 and 3.31 is included. 13. <input checked="" type="checkbox"/> A FIRST preliminary amendment. 14. <input type="checkbox"/> A SECOND or SUBSEQUENT preliminary amendment. 15. <input type="checkbox"/> A substitute specification. 16. <input type="checkbox"/> A change of power of attorney and/or address letter. 17. <input type="checkbox"/> A computer-readable form of the sequence listing in accordance with PCT Rule 13ter.2 and 35 U.S.C. 1.821 - 1.825. 18. <input type="checkbox"/> A second copy of the published international application under 35 U.S.C. 154(d)(4). 19. <input type="checkbox"/> A second copy of the English language translation of the international application under 35 U.S.C. 154(d)(4). 20. <input type="checkbox"/> Other items or information:					

US APPLICATION NO. (if known, enter 37 CFR 1.53) <b>097/856200</b>	INTERNATIONAL APPLICATION NO. <b>PCT/US98/23905</b>	ATTORNEY'S DOCKET NUMBER <b>54203-H-PCT-US/JPW/SHS</b>
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21. <input checked="" type="checkbox"/> The following fees are submitted: <b>BASIC NATIONAL FEE (37 CFR 1.492 (a) (1) - (5)):</b> Neither international preliminary examination fee (37 CFR 1.482) nor international search fee (37 CFR 1.445(a)(2)) paid to USPTO and International Search Report not prepared by the EPO or JPO. .... <b>\$1000.00</b>  International preliminary examination fee (37 CFR 1.482) not paid to USPTO but International Search Report prepared by the EPO or JPO ..... <b>\$860.00</b>  International preliminary examination fee (37 CFR 1.482) not paid to USPTO but international search fee (37 CFR 1.445(a)(2)) paid to USPTO ..... <b>\$710.00</b>  International preliminary examination fee (37 CFR 1.482) paid to USPTO but all claims did not satisfy provisions of PCT Article 33(1)-(4) ..... <b>\$690.00</b>  International preliminary examination fee (37 CFR 1.482) paid to USPTO and all claims satisfied provisions of PCT Article 33(1)-(4) ..... <b>\$100.00</b> <b>ENTER APPROPRIATE BASIC FEE AMOUNT =</b>	<table border="1" style="width:100%; border-collapse: collapse;"> <tr> <th colspan="2" style="text-align: left;">CALCULATIONS PTO USE ONLY</th> </tr> <tr> <td style="width:50%;"></td> <td style="width:50%;"></td> </tr> <tr> <td></td> <td style="text-align: right;">\$ 710</td> </tr> <tr> <td colspan="2">Surcharge of \$130.00 for furnishing the oath or declaration later than <input type="checkbox"/> 20 <input type="checkbox"/> 30 months from the earliest claimed priority date (37 CFR 1.492(e)).</td> </tr> <tr> <td>CLAIMS</td> <td>NUMBER FILED</td> </tr> <tr> <td>Total claims</td> <td>32 - 20 = 12</td> </tr> <tr> <td>Independent claims</td> <td>13 - 3 = 10</td> </tr> <tr> <td colspan="2">MULTIPLE DEPENDENT CLAIM(S) (if applicable)</td> </tr> <tr> <td colspan="2">TOTAL OF ABOVE CALCULATIONS =</td> </tr> <tr> <td colspan="2"><input type="checkbox"/> Applicant claims small entity status. See 37 CFR 1.27. The fees indicated above are reduced by 1/2.</td> </tr> <tr> <td colspan="2">SUBTOTAL =</td> </tr> <tr> <td colspan="2">Processing fee of \$130.00 for furnishing the English translation later than <input type="checkbox"/> 20 <input type="checkbox"/> 30 months from the earliest claimed priority date (37 CFR 1.492(f)).</td> </tr> <tr> <td colspan="2">TOTAL NATIONAL FEE =</td> </tr> <tr> <td colspan="2">Fee for recording the enclosed assignment (37 CFR 1.21(h)). The assignment must be accompanied by an appropriate cover sheet (37 CFR 3.28, 3.31). \$40.00 per property +</td> </tr> <tr> <td colspan="2">TOTAL FEES ENCLOSED =</td> </tr> <tr> <td colspan="2">Amount to be refunded:</td> </tr> <tr> <td colspan="2">charged:</td> </tr> </table>	CALCULATIONS PTO USE ONLY					\$ 710	Surcharge of \$130.00 for furnishing the oath or declaration later than <input type="checkbox"/> 20 <input type="checkbox"/> 30 months from the earliest claimed priority date (37 CFR 1.492(e)).		CLAIMS	NUMBER FILED	Total claims	32 - 20 = 12	Independent claims	13 - 3 = 10	MULTIPLE DEPENDENT CLAIM(S) (if applicable)		TOTAL OF ABOVE CALCULATIONS =		<input type="checkbox"/> Applicant claims small entity status. See 37 CFR 1.27. The fees indicated above are reduced by 1/2.		SUBTOTAL =		Processing fee of \$130.00 for furnishing the English translation later than <input type="checkbox"/> 20 <input type="checkbox"/> 30 months from the earliest claimed priority date (37 CFR 1.492(f)).		TOTAL NATIONAL FEE =		Fee for recording the enclosed assignment (37 CFR 1.21(h)). The assignment must be accompanied by an appropriate cover sheet (37 CFR 3.28, 3.31). \$40.00 per property +		TOTAL FEES ENCLOSED =		Amount to be refunded:		charged:	
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a. ☐ A check in the amount of \$ \_\_\_\_\_ to cover the above fees is enclosed.

b. ☒ Please charge my Deposit Account No. 03-3125 in the amount of \$ 1726 to cover the above fees. A duplicate copy of this sheet is enclosed.

c. ☒ The Commissioner is hereby authorized to charge any additional fees which may be required, or credit any overpayment to Deposit Account No. 03-3125. A duplicate copy of this sheet is enclosed.

d. ☐ Fees are to be charged to a credit card. **WARNING:** Information on this form may become public. **Credit card information should not be included on this form.** Provide credit card information and authorization on PTO-2038.

**NOTE:** Where an appropriate time limit under 37 CFR 1.494 or 1.495 has not been met, a petition to revive (37 CFR 1.137 (a) or (b)) must be filed and granted to restore the application to pending status.

SEND ALL CORRESPONDENCE TO: <b>John P. White, Esq.</b> <b>Cooper &amp; Dunham LLP</b> <b>1185 Avenue of the Americas</b> <b>New York, New York 10036</b>	<div style="text-align: center;"> </div> <hr/> SIGNATURE <b>John P. White</b> <hr/> NAME <b>Spencer Schneider</b> <hr/> Reg. No. 28,678 Reg. No. 45,923 <hr/> REGISTRATION NUMBER
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09/856200  
JC18 Rec'd PCT/PTO 1 4 MAY 2001

Dkt. 54203-H-PCT/JPW/SHS

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicants : Peter D. Kwong et al.  
Serial No. : Not Yet Known (U.S. National Stage of  
PCT/US98/23905, filed 10 November 1998)  
Filed : Herewith  
For : CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY  
VIRUS ENVELOPE GLYCOPROTEIN gp120, COMPOUNDS  
INHIBITING CD4-gp120 INTERACTION, COMPOUNDS  
INHIBITING CHEMOKINE RECEPTOR-gp120  
INTERACTION, MIMICS OF CD4 AND gp120 VARIANTS

1185 Avenue of the Americas  
New York, New York 10036  
May 7, 2001

Assistant Commissioner for Patents  
Washington, D.C. 20231

PRELIMINARY AMENDMENT

Please amend the subject application as follows:

In the specification:

On page 1, line 1, after the title, please delete the paragraph beginning "This application is a..." and insert the following paragraph:

--This application is a national stage entry filed under 35 U.S.C. §371 of PCT International Application No. PCT/US98/23905, filed November 10, 1998, which is a continuation-in-part and claims the benefit of U.S. Serial No. 09/100,631, filed June 18, 1998, U.S. Serial No. 09/100,763, filed June 18, 1998, U.S. Serial No. 09/100,529, filed June 18, 1998, U.S. Serial No. 09/100,762, filed June 18, 1998,

Applicants : Peter D. Kwong et al.  
Serial No. : Not Yet Known  
Filed : Herewith  
Page 2

U.S. Serial No. 09/100,521, filed June 18, 1998 and claims the benefit of U.S. Serial No. 08/976,741, filed November 24, 1997, U.S. Serial No. 08/966,987, filed November 10, 1997, U.S. Serial No. 08/967,403, filed November 10, 1997, U.S. Serial No. 08/966,932, filed November 10, 1997, and U.S. Serial No. 08/967,148, filed November 10, 1997, the contents of which are incorporated by reference into this application.-

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In the claims:

Please cancel claims 2-20, 22-26, 29-32, 35, 39-41, 43, 50-52, 54, 60, 62-79, 82, 87-89, 92-93, 95-96 without disclaimer or prejudice to applicants' right to pursue the subject matter of these claims in a later-filed application. Please amend claims 33, 44, 46, 55, 57, 90 and 94 under the provisions of 37 C.F.R. § 1.121(c) as follows. A marked up version of the amended claims wherein the deleted material is in brackets and the inserted material is underlined is attached hereto as Exhibit 1.

- 33. (Amended) The compound identified by the method of claim 27.
- 44. (Amended) The compound identified by the method of claim 37.
- 46. (Amended) A composition comprising the compound of claim 44 and a suitable carrier.--
- 55. (Amended) The compound identified by the method of claim





Respectfully submitted,

John P. White  
Registration No. 28,678  
Attorneys for Applicant(s)  
Spencer H. Schneider  
Registration No. 45,923  
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(212) 278-0400

Applicants : Peter D. Kwong et al.  
 Serial No. : Not Yet Known  
 Filed : Herewith  
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**EXHIBIT 1**

- 33. (Amended) The compound identified by the method of claim  
 [32] 27.
- 44. (Amended) The compound identified by the method of claim  
 [43] 37.
- 46. (Amended) A composition comprising the compound of claim  
 44 [or 45] and a suitable carrier.--
- 55. (Amended) The compound identified by the method of claim  
 [54] 48.--
- 57. (Amended) A composition comprising the compound of claim  
 55 [or 56] and a suitable carrier.--
- 90. (Amended) A vaccine comprising the variant of claim 86  
 [,87 or 88].
- 94. (Amended) An antibody against the variant of claim 86  
 [,87 or 88].

09856200.010303

Applicant or Patentee: Peter D. Kwong, et al. Attorney's  
Serial or Patent No.: 09/856,200 Docket No: 54203-H-PCT-US  
Filed or Issued: November 10, 1998 JPW/AJM/HA  
Title of Invention or Patent: CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN gp120 COMPOUND INHIBITING CD-4gp120 INTERACTION, COMPOUND INHIBITING CHEMOKINE RECEPTOR gp120 INTERACTION, MIMICS OF CD4 AND gp120 VARIANTS

**VERIFIED STATEMENT (DECLARATION) CLAIMING  
SMALL ENTITY STATUS UNDER 37 C.F.R. §1.9(f)  
AND §1.27(d) - NONPROFIT ORGANIZATION**

I hereby declare that I am an official empowered to act on behalf of the nonprofit organization identified below:

Name of Organization: The Trustees of Columbia University  
In the City of New York  
Address of Organization: Broadway and West 116th Street  
New York, New York 10027

**TYPE OF ORGANIZATION:**

☒ UNIVERSITY OR OTHER INSTITUTION OF HIGHER EDUCATION  
☐ TAX EXEMPT UNDER INTERNAL REVENUE SERVICE CODE 26 U.S.C. §§501(a) and 501(c)(3)  
☐ NONPROFIT SCIENTIFIC OR EDUCATIONAL UNDER STATUTE OF STATE OF THE UNITED STATES OF AMERICA  
NAME OF STATE: \_\_\_\_\_  
CITATION OF STATUTE: \_\_\_\_\_  
☐ WOULD QUALIFY AS TAX EXEMPT UNDER INTERNAL REVENUE SERVICE CODE 26 U.S.C. §§501(a) and 501(c)(3) IF LOCATED IN THE UNITED STATES OF AMERICA  
☐ WOULD QUALIFY AS NONPROFIT SCIENTIFIC OR EDUCATIONAL UNDER STATUTE OF STATE OF THE UNITED STATES OF AMERICA IF LOCATED IN THE UNITED STATES OF AMERICA  
NAME OF STATE: \_\_\_\_\_  
CITATION OF STATUTE: \_\_\_\_\_

I hereby declare that the nonprofit organization identified above qualifies as a nonprofit organization as defined in 37 C.F.R. §1.9(e)\* for purposes of paying reduced fees under 35 U.S.C. §41(a) and 41(b), with regard to the invention entitled CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN gp120 COMPOUND INHIBITING CD4-gp120 INTERACTION, COMPOUNDS INHIBITING CHEMOKINE RECEPTOR gp120 INTERACTION, MIMICS OF CD4-gp120 VARIANTS by inventor(s) Peter D. Kwong, Wayne A. Hendrickson, Joseph G. Sodroski, Richard T. Wyatt described in:

☐ the specification filed herewith  
☒ application serial no. 09/856,200 filed November 10, 1998  
☐ patent no. \_\_\_\_\_ issued \_\_\_\_\_

I hereby declare that rights under contract or law have been conveyed to and remain with the nonprofit organization with regard to the above identified invention.

If the rights held by the nonprofit organization are not exclusive each individual, concern, or organization known to have rights to the invention is listed below<sup>a</sup> and no rights to the invention are held by any person, other than the inventor, who could not qualify as a small business concern under 37 C.F.R. §1.9(d)\* or a nonprofit organization under 37 C.F.R. 1.9(e)\*

<sup>a</sup> NOTE: Separate verified statements are required from each person, concern, or organization having rights to the invention averring to their status as small entities. 37 C.F.R. §1.27.

Name: \_\_\_\_\_  
Address: \_\_\_\_\_


☐ Individual ☐ Small Business Concern ☐ Nonprofit Organization

**Small Entity/Nonprofit**

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I acknowledge the duty to file, in this application or patent, notification of any change in status resulting in loss of entitlement to small entity status prior to paying, or at the time of paying, the earliest of the issue fee or any maintenance fee due after the date on which status as a small entity is no longer appropriate. 37 C.F.R. §1.28(b)\*.

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under 18 U.S.C. §1001, and that such willful false statements may jeopardize the validity of the application, any patent issuing thereon, or any patent to which this verified statement is directed.

Name of Person Signing: Michael J. Cleare, Ph.D.  
 Title In Organization: Executive Director - Columbia Innovation Enterprise  
 Address: Columbia University, Engineering Terrace - Suite 363  
Amsterdam Avenue & West 120th Street, New York, New York 10027  
 Signature:   
 Date Of Signature: 12/28/02

CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY VIRUS  
ENVELOPE GLYCOPROTEIN gp120, COMPOUNDS INHIBITING  
CD4-gp120 INTERACTION, COMPOUNDS INHIBITING  
CHEMOKINE RECEPTOR-gp120 INTERACTION,  
MIMICS OF CD4 AND gp120 VARIANTS

This application is a continuation-in-part of U.S. Serial No. 09/100,631, filed June 18, 1998, a continuation-in-part of U.S. Serial No. 08/976,741, filed November 24, 1997, U.S. Serial No. 09/100,763, 5 filed June 18, 1998, a continuation-in-part of U.S. Serial No. 08/966,987, filed November 10, 1997, U.S. Serial No. 09/100,529, filed June 18, 1998, a continuation-in-part of U.S. Serial No. 08/967,403, filed November 10, 1997, U.S. Serial No. 09/100,762, 10 filed June 18, 1998, a continuation-in-part of U.S. Serial No. 08/966,932, filed November 10, 1997, U.S. Serial No. 09/100,521, filed June 18, 1998 a continuation-in-part of U.S. Serial No. 08/967,148, filed November 10, 1997. The contents of the above- 15 identified application are incorporated into this application by reference.

The invention disclosed herein was made with United States Government support under National Institute of 20 Health Grant Nos. Al 31783, Al 39420, Al 28691, CA 06516, Al 41851, Al 40895, GM 5-20394 and CUID 511168. Accordingly, the United States Government has certain rights in this invention.

25 Various references are referred to within this application. Disclosures of these publications in their entireties are hereby incorporated by reference into this application to more fully describe the state of the art to which this invention pertains.

30

Background of the Invention

During the first thirty years of protein

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crystallization, the standard conceptual practice was to treat the protein as a fixed constant and screen it through a multitude of crystallization conditions. Advances in this approach has led to the development of crystallization robots capable of testing thousands of conditions (1,2). While this approach has had success, it fails for many interesting proteins.

One of these is the Human Immunodeficiency Virus (HIV)-1 envelope glycoprotein, gp120. HIV induces acquired immunodeficiency syndrome (AIDS) in humans (3,4). The gp120 glycoprotein helps to mediate virus entry into cells through sequential recognition of two cellular receptors of the human host, CD4 (5,6), and a chemokine receptor (primarily CXCR-4 or CCR-5, depending on viral strain) (7-12). These high affinity interactions are attractive targets for mimetic drug design. Although the structure of the gp120-binding domain of CD4 and the identity of residues critical to its interaction with gp120 have been known for several years (13,14), this has not been sufficient for design of potent antagonists (15-17). As the major virus-specific antigen accessible to neutralizing antibodies, knowledge of the gp120 structure could also impact considerably on vaccine design.

The gp120 protein has been an obvious target for structural investigation, and quantities of pure soluble protein have been available for several years, a byproduct in part from vaccine trials. Nevertheless, despite considerable effort, it has resisted crystallographic analysis for more than a decade.

The mature gp120 glycoproteins of different HIV-1 strains have approximately 470-490 amino acids (18).

Extensive N-linked glycosylation at approximately 20-25 sites accounts for roughly half its mass (18,19). Sequences from many different viral isolates show that it contains five conserved regions (C1-C5) and five  
5 variable regions (V1-V5): (18, 20) and nine conserved disulfide bridges (19). Except for limited N- and C-terminal cleavage, proteolytic digestion does not reveal a sub-domain structure. Indeed, even after extensive  
10 proteolytic cleavage, the unreduced protein runs near its native molecular weight on SDS-PAGE (Peter D. Kwong: unpublished data). Some of the variable regions, the V3 loop in particular, appear to be conformationally variable. Conformational change is also evidenced by  
15 shedding, the CD4-induced dissociation of gp120 from the surface of the virus, and by ligand-induced variations in monoclonal antibody binding (21,22). These changes may be related to the functional role of gp120 in virus entry.

20 The extensive glycosylation and conformational heterogeneity of gp120 suggested that merely screening the protein through ever more exotic crystallization conditions would not produce well-diffracting crystals. We therefore adopted a fundamentally different approach,  
25 which we term variational crystallization. This approach employed on radical modification of the protein surface, primarily to reduce heterogeneity, but also as a means of varying potential crystallization lattice contacts. An interactive cycle, involving different  
30 biochemical and molecular biological techniques, was used to detect and remove chemical and conformational heterogeneity. In addition, protein ligands, such as CD4 and the Fabs of monoclonal antibodies, were used to restrict conformational mobility. Progressive trials of  
35 18 different gp120 crystallization variants yielded six



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different crystals. This paradigm of crystallization, with a focus on protein modification rather than on crystallization screening, may aid in the structural analysis of other conformationally complex proteins.

**Summary of the Invention**

The subject invention provides a crystal suitable for X-ray diffraction comprising a polypeptide having an amino acid sequence of a portion of a Human Immunodeficiency Virus envelope glycoprotein gp120, wherein the amino acid sequence is at least 100 amino acids in length.

The subject invention also provides the above-described crystals, which effectively diffract X-rays for determination of the atomic coordinates of the polypeptide to a resolution of 2.5 angstroms or better than 2.5 angstroms.

The subject invention also provides the above-described crystals, wherein the crystal is arranged in a space group  $P222_1$ , so as to form a unit cell of dimensions  $a=71.6 \text{ \AA}$ ,  $b=88.1 \text{ \AA}$ ,  $c=196.7 \text{ \AA}$ , and which effectively diffracts x-rays for determination of the atomic coordinates of the gp120 to a resolution of 2.5  $\text{\AA}$  or better.

The subject invention additionally provides a method for producing a crystal suitable for X-ray diffraction comprising: (a) deglycosylating a polypeptide having amino acid sequence of a portion of a gp120 wherein said portion is produced by deleting or replacing part of the gp120 to reduce the surface loop flexibility; (b) contacting the polypeptide with a ligand so as to form a complex which exhibits restricted conformational mobility; and (c) obtaining crystal from the complex so formed to produce a crystal suitable for X-ray diffraction.

The subject invention also provides the above-described methods, wherein the V1, V2, or V3 loop of the gp120

contained in the polypeptide are partially truncated, deleted or replaced.

5 The subject invention also provides a method for identifying a compound capable of binding to a portion of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining a binding site on the portion of gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal  
10 comprising the portion of gp120; and (b) determining whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the gp120.

15 This invention also provides a method of inhibiting the interaction of HIV-gp120 with CD4 which comprises administering to a mammal in need thereof a compound capable of disrupting two or more of the contacts between gp120 and CD4 as set forth in Figure 54.

20 This invention also provides a method for identifying a compound capable of binding to the CD4 binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the CD4 binding site on the  
25 gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of gp120 capable of binding to CD4; and (b) determining whether a compound would fit into the binding site, a  
30 positive fitting indicating that the compound is capable of binding to the CD4 binding site of the gp120.

This invention also provides a method for designing a compound capable of binding to the CD4 binding site of  
35 Human Immunodeficiency Virus envelope glycoprotein gp120

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comprising: (a) determining the CD4 binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of  
5 gp120 capable of binding to CD4; and (b) designing a compound to fit the CD4 binding site.

This invention also provides a method of inhibiting Human Immunodeficiency Virus infection in a subject  
10 comprising administering effective of amount of the above-described composition to the subject.

This invention provides a method for identifying a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the  
15 chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having the amino acid sequence of a portion of gp120 capable of  
20 binding to the chemokine receptor; and (b) determining whether a compound would fit into the binding site, a positive fit indicating that the compound is capable of binding to the chemokine receptor binding site of the  
25 gp120.

This invention also provides a method for designing a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the  
30 chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having the amino acid sequence of a portion of gp120 capable of  
35 binding to the chemokine receptor; and (b) designing a

compound to fit the chemokine receptor binding site.

This invention also provides the above-described methods, wherein the crystal further comprises a  
5 chemokine receptor, a second polypeptide having amino acid sequence of a portion of chemokine receptor, an antibody or a Fab capable of binding to the chemokine receptor binding site or a compound known to be capable of binding to the chemokine receptor binding site, bound  
10 to the polypeptide.

This invention further provides a method of inhibiting the interaction of HIV-gp120 with chemokine receptor which comprises administering to a mammal in need  
15 thereof a compound capable of disrupting two or more of the contacts between gp120 and chemokine receptor as set forth in Figure 55, thereby inhibiting the interaction of HIV-gp120 with chemokine receptor.

20 This invention provides a substance mimicking the gp120-binding domain of CD4 wherein the size of the residue or analog thereof at position 43 is bigger than the size of a phenylalanine so as to increase the affinity for human immunodeficiency virus envelope glycoprotein gp120.

25 This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof larger than 10 Å across its longest dimension.

30 This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof, wherein the residue's longest dimension is longer than phenylalanine's longest  
35 dimension.

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This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof larger than 15 Å across its longest dimension.

5

This invention also provides the above-described substances, wherein the modification involves replacement of the residue at position 43 with a cysteine.

10

This invention also provides the above-described substances, wherein the modification involves replacement of the residue at position 43 with a tyrosine.

15

This invention further provides a pharmaceutical composition capable of inhibiting cell entry by HIV, comprising (a) an effective amount of the substance of claim 1; and (b) a pharmaceutically acceptable carrier.

20

This invention further provides a method of inhibiting cell entry by HIV, comprising contacting the cells with an effective amount of the above-described substances, thereby inhibiting cell entry by HIV.

25

This invention further provides a method of treating or preventing HIV infection in a subject, comprising administering to the subject an effective amount of the above-described substances, thereby treating or preventing HIV infection.

30

The subject invention provides a variant of gp120 which presents a hidden, conserved, neutralization epitope.

35 The subject invention also provides a composition

-10-

comprising a variant of gp120 which presents a hidden, conserved, neutralization epitope and a suitable carrier.

- 5 The subject invention further provides a vaccine comprising a variant of gp120 which presents a hidden conserved, neutralization epitope and a suitable carrier.
- 10 The subject invention also provides an antibody induced by a vaccine comprising a variant of gp120.

**Brief Description of the Figures****Figures for the First Series of Experiments****Figure 1**

5 Computer-generated ribbon drawing of the tertiary structure of CD4, gp120, and Fab 17b interacting. CD4 is in the top left, gp120 is toward the right, and Fab 17b is in the bottom left of the figure.

**Figure 2**

10 Illustration of the locations of CD4, gp120, and Fab 17b in the computer-generated ribbon drawing of figure 1.

**Figure 3**

Photomicrographs of crystals containing HIV-1 gp120. Crystal types A-F are shown and correspond to the crystal types described in the text and Tables 3 and 4. 15 The photomicrograph in A is at twice the magnification. The bar in A corresponds to 25  $\mu\text{m}$  (50  $\mu\text{m}$  for B-F).

**Figure 4**

Polyacrylamide gel electrophoresis (PAGE) of the ternary complex crystals (Type E). A cluster of crystals 20 (0.4x0.1x0.05mM) was washed four times with 1  $\mu\text{l}$  of reservoir solution and dissolved in 3  $\mu\text{l}$  of loading buffer and analyzed by SDS-PAGE on a 8-25% gradient gel (Pharmacia Phast system). Lane 1, 2.5 ug of ternary complex purified by gel filtration. The top band is the 25 deglycosylated  $\Delta 82\Delta V1/2^*\Delta V3\Delta C5$  gp120, the next two bands are the alkylated and reduced heavy and light chains respectively of the Fab 17b, and the bottom band is the two-domain sCD4 (D1D2). Lane 2, standards: 94, 67, 43 (diffuse), 30, 20, and 14. Lane 3, supernant from the 30 crystallization droplet. Lane 4, last wash of crystals. Lane 5, dissolved crystals. The gel is silver stained.

**Figure 5 A and B**

Crystals formed under condition one described in Table 7.

35 **Figure 6**



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- Crystals formed under condition two described in Table 7.
- Figure 7
- Crystals formed under condition three described in Table 7.
- Figure 8
- Crystals formed under condition four described in Table 7.
- Figure 9
- Crystals formed under condition five described in Table 7.
- Figure 10
- Crystals formed under condition six described in Table 7.
- Figure 11
- Crystals formed under condition seven described in Table 7.
- Figure 12
- Crystals formed under condition eight described in Table 7.
- Figure 13
- Crystals formed under condition nine described in Table 7.
- Figure 14
- Crystals formed under condition ten described in Table 7.
- Figure 15
- Crystals formed under condition eleven described in Table 7.
- Figure 16
- Crystals formed under condition twelve described in Table 7.
- Figure 17
- Crystals formed under condition thirteen described in Table 7.

Figure 18

Crystals formed under condition fourteen described in Table 7.

Figure 19

- 5 Crystals formed under condition fifteen described in Table 7.

Figure 20

Crystals formed under condition sixteen described in Table 7.

- 10 Figure 21

Crystals formed under condition seventeen described in Table 7.

Figure 22

- 15 Crystals formed under condition eighteen described in Table 7.

Figure 23

Crystals formed under condition nineteen described in Table 7.

Figure 24

- 20 Crystals formed under condition twenty described in Table 7.

Figure 25

Crystals formed under condition twenty-one described in Table 7.

25

**Figures for the Second Series of Experiments**Figures 26A and 26B

- 30 The HIV-1 entry process. The trimeric HIV-1 envelope glycoproteins, anchored in the viral membrane, are depicted, with gp120 in the lower right and gp41 in the upper right. For simplicity, the gp120 variable loops are not shown, but would extend over the outer surface of the envelope glycoprotein complex. The receptors on the target cell, CD4 and chemokine receptor, are also
- 35 shown. The structures of gp120, gp41, and CD4 are

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adapted from available X-ray crystallographic studies (5,20,21), whereas the chemokine receptor model is hypothetical.

Figure 27

5 The HIV-1 gp120 surface.

Figure 27A

The molecular surface of the HIV-1 gp120 core (20) is shown, with the arrow pointing towards the viral membrane. The inner domain, believed to interact with  
10 gp41, and the outer domain, which is probably exposed on the assembled trimer, are on the left and right, respectively. The gp120 surface occluded by CD4 is shown and the gp120 region thought to be involved in chemokine receptor binding (27) is also shown. The  
15 location of the base of the V3 loop is shown.

Figure 27B

Conserved gp120 neutralization epitopes are shown on the gp120 core, which is oriented identically to that in Figure 16A. The location of the epitopes was deduced  
20 from mutagenic analysis (45,46,48).

Figure 27C

The approximate location of gp120 structures (20) that contribute to protection from antibody responses is shown. The major variable loops (V2, V3, and V4), the  
25 V5 region and the sites of N-linked glycosylation are shown.

Figure 16D

The relationship of different surfaces of the gp120 core to the antibody response generated by the gp120  
30 glycoprotein is depicted. The surface of gp120 that interacts with neutralizing antibodies (32) is shown, spans the inner and outer domains, and includes the V2 and V3 variable loops (not shown). The surface of gp120 that interacts with non-neutralizing antibodies is  
35 located on the inner domain, and includes gp41-

-15-

interactive N- and C-terminal gp120 regions (not shown). The heavily glycosylated surface of the gp120 outer domain, which appears to be minimally immunogenic, is also shown.

5

### **Figures for the Third Series of Experiments**

#### Figure 28

Overall structure. The ribbon diagram shows gp120, the N-terminal two domains of CD4, and the Fab 17b (light chain) and (heavy chain). The sidechain of Phe 43 on CD4 is also shown. The prominent CDR3 loop of the 17b heavy chain is evident in this orientation. Although the complete N- and C- termini of gp120 are missing, the positions of the gp120 termini are consistent with the proposal that gp41, and hence the viral membrane, is located towards the top of the diagram. This would position the target membrane at the diagram base. The vertical dimension of gp120 in this orientation is roughly 50 Å. Precisely perpendicular views of gp120 are shown in Figures 29 and 30. Drawn with RIBBONS<sup>49</sup>.

#### Figure 29

Structure of core gp120. The orientation of gp120 in each of the panels shown in this figure is related to Figure 17 by a 90° rotation about a vertical axis. Thus the viral membrane would be oriented above, the target membrane below, and the C-terminal tail of CD4 coming out of the page. In this view, we describe the left portion of core gp120 as the "inner" domain, the right portion as the "outer" domain, and the 4-stranded sheet at the bottom left of gp120 as the "bridging sheet." The bridging sheet ( $\beta 3$ ,  $\beta 2$ ,  $\beta 21$ ,  $\beta 20$ ) can be seen packing primarily over the inner domain, although some surface residues of the outer domain, e.g. Phe 382, reach in to form part of its hydrophobic core.

#### Figure 29A

35

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Ribbon diagram. Helices and  $\beta$ -strands are depicted. strand  $\beta 15$  makes an antiparallel  $\beta$ -sheet alignment with strand C'' of CD4. The dashed line to the right of the diagram represents the disordered V4 loop. Selected parts of the structure are labeled.

#### Figure 29B

Secondary structure diagram. The schematic is arranged to coincide with the orientation of Figures 29A and 29C. Helices are shown as corkscrews and labeled  $\alpha 1$ - $\alpha 5$ .  $\beta$ -strands are shown as arrows: black and labeled represent the 25  $\beta$ -strands of core gp120; gray and unlabeled represent the continuation of hydrogen bonding across a sheet; white and labeled represents the C'' strand of CD4. Spatial proximity between neighboring strands implies mainchain hydrogen bonding. Loops are labeled  $\zeta A$ - $\zeta F$  and V1-V5. The labels of loops with high sequence variability are circled. Assignment of secondary structure was accomplished with the Kabsch and Sander algorithm except for  $\beta 4$  and  $\beta 8$ , which are both interrupted mid-strand by sidechain-backbone hydrogen bonds,  $\beta 9$ ,  $\beta 15$ , and  $\beta 25a$ , all of which have angles or hydrogen bonds which are slightly non-standard, and  $\alpha 4$ , which hydrogen bonds as a 3-10 helix with the final residue in  $\beta$ -conformation.

#### Figure 29C

Stereo plot of an  $\alpha$ -carbon trace. Every 10th C $\alpha$  is marked with a filled circle, and every twentieth residue is labeled. Disulfide connections are depicted as ball and stick. Shown are ordered residues, 90-396 and 410-492.

#### Figure 29D

Structure-based sequence alignment. Shown are the sequences of "HIV-1 B" (core gp120 from clade B, strain HXBc2 used in these studies), "C" (HIV-1 clade C, strain UG268A2), "O" (HIV-1 clade O, strain ANT70),

-17-

"HIV-2"(strain ROD), and "SIV"(African green monkey isolate, clone GRI-1). The secondary structure assignments are shown as arrows and cylinders, with (x) denoting residues which are disordered in the present structure. The "gars" sequence at the N-terminus and the "gag" sequence in the V1/V2 and V3 loops are consequences of the gp120 truncation. Solvent accessibility is indicated for each residue by an open circle if the fractional solvent accessibility is greater than 0.4, a half-closed circle if 0.1 to 0.4, and a closed circle if less than 0.1. Sequence variability observed among primate immunodeficiency viruses is indicated below the solvent accessibility by the number of horizontal hash marks: 1 mark, residues conserved among all primate immunodeficiency viruses; 2 marks, conserved among all HIV-1 isolates; 3 marks, exhibits moderate variation among HIV-1 isolates; and 4 marks, exhibits significant variability among HIV-1 isolates. In accessing conservation, all single atom changes were permitted as well as larger substitutions if the character of the sidechain was conserved (e.g. K to R or F to L). N-linked glycosylation is indicated by "m" for the high mannose additions and "c" for the complex additions observed in mammalian cells (6). Residues of gp120 in direct contact with CD4 are indicated by "\*". Direct contact is a more restrictive criterion of interaction than the often used loss of solvent accessible surface; residues of gp120 which show loss of solvent accessible surface but are not in direct contact are 123, 124, 126, 257, 278, 282, 364, 471, 475, 476 and 477. Parts (a) and (b) were drawn with MOLSCRIPT (P. J. Kraulis).

Figure 30

CD4-gp120 interactions.

Figure 30A

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Ribbon diagram of gp120 binding to CD4. Residue Phe 43 of CD4 is also depicted reaching into the heart of gp120. From this orientation the recessed nature of the gp120 binding pocket is evident.

5 Figure 30B

Electron density in the Phe 43 cavity. The 2Fo-Fc electron density map at 2.5Å, 1.1σ contour, is shown. The orientation is the same as in (a). The foreground has been clipped for clarity removing the overlying β24-α5 connection. In the upper middle of the picture is the central unidentified density. At the bottom of the picture, Phe 43 of CD4 can be seen reaching up to contact the cavity. Moving clockwise around the cavity, the gp120 residues are Trp 427 (with its indole ring partially clipped by foreground slabbing), Trp 112, Val 15 255, Thr 257, Glu 370 (packing under the Phe 43 ring), Ile 371, and Glu 368 (partially clipped in the bottom right corner). Hydrophobic residues lining the back of the cavity can be partially glimpsed around the central 20 unidentified density.

Figure 30C

Electrostatic surface of CD4 and gp120. The electrostatic potential is displayed at the solvent accessible surface, which is shaded according to the 25 local electrostatic potential. The slight "puffiness" of the surface arises from the enlarged nature of the solvent accessible surface relative to the standard molecular surface. On the right, the gp120 surface is shown in an orientation similar to that of Figures 29A and 29C, but rotated ~20° around a vertical axis to 30 depict the recessed binding pocket more clearly. A thin yellow Cα worm of CD4 is shown to aid in orientation. On the left, the CD4 surface is shown, rotated relative to the gp120 panel by an exact 180° rotation about the 35 vertical axis shown. A thin red Cα worm of gp120 is

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shown.

Figure 30D

CD4-gp120 contact surface. On the right, the gp120 surface is shown with the surface within 3.5 Å of CD4 (surface-to-atom center distance). This effectively creates an "imprint" of CD4 on the displayed gp120 surface. On the left (180° rotation), the corresponding CD4 surface and gp120 "imprint" is also shown.

Figure 30E

CD4-gp120 mutational "hot-spots." On the right, the surface of gp120 is shown with the surface of gp120 residues shown by substitution to affect CD4 binding highlighted: substantial effect -- residues 257, 368, 370 and 427; moderate effect -- residue 457. Also depicted is the surface of the large water-filled cavity at the CD4-gp120 interface. On the left (180° rotation), residues important for gp120 binding are shown on the CD4 surface: substantial effect -- residues 43 and 59; moderate effect -- residues 29, 35, 44, 46, 47.

Figure 30F

Sidechain/mainchain contribution to the gp120 surface. The orientation is the same as the right panel of Figures 30C-30E, and below (Figure 30G), and allows for direct comparison of the CD4-gp120 contact surface. A striking surface concentration of mainchain atoms is seen in the regions corresponding to the CD4 "imprint."

Figure 30G

Sequence variability mapped to the gp120 surface. The sequence variability observed among primate immunodeficiency viruses (Figure 29D) is depicted mapped onto the gp120 surface. Also shown is the carbohydrate: N-acetylglucosamine and fucose residues present in the structure; Asn-proximal N-acetylglucosamines modeled at residues 88, 230, 241, 356, 397, 406, 462. Much of the carbohydrate (22 residues) is hidden on the back side of



the outer domain.

Figure 30H

Phe 43 cavity. The surface of the Phe 43 cavity is shown, buried in the heart of gp120. A worm representation of gp120 shows the three stretches that are incorrectly predicted by secondary structure prediction: the  $\zeta$ B loop, bending around the top of the cavity, strands  $\beta$ 20- $\beta$ 21 just below the cavity, and strand  $\beta$ 15, slightly more distal to the cavity right. The orientation shown here is the same as for the gp120 surfaces in Figure 30C-G.

Figure 30I

Schematic of the CD4-gp120 interface. This schematic of the entire interface shows six discrete segments of gp120 (solid black line) interacting with CD4 (double line). To aid in orientation, secondary structural elements are labeled, as are representative contact residues from each segment of gp120. Arrows indicate mainchain direction. The sidechain of Phe 43 is also shown. The orientation shown is similar to Figure 30A and 30B.

Figure 30J

Schematic of gp120 contacts around Phe 43 and Arg 59 of CD4. Residues on gp120 involved in direct contact with Phe 43 or Arg 59 are depicted. Electrostatic interactions are depicted as dashed lines. Hydrophobic interactions are found between Phe 43 (CD4) and Trp 427, Glu 370, Gly 473, and Ile 371 (all from gp120) and between Arg 59 (CD4) and Val 430 (gp120). The orientation is similar to Figure 30A, 30B, and 30I, but has been rotated for clarity. Sidechains of Phe 43 and Arg 59 as well as those portions of gp120 sidechains which interact with these crucial CD4 residues are drawn with bold lines.

35 (Figure 30A was drawn with RIBBONS<sup>49</sup>, Figure 30B with the

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program O<sup>47</sup>, and Figures 30B-G with GRASP<sup>50</sup>.)

Figure 31

Neutralizing antibody 17b-gp120 interface.

Figure 31A

- 5 Worm diagram of Fab 17b and gp120. The Fab 17b is shown binding to gp120. The orientation shown is the same as in Figures 29A and 29C.

Figure 31B

- 10 Contact surface and V3 loop. The surface of gp120 is shown with any surface within 3.5 Å of Fab 17b (surface-to-atom center) and the surface of the V3 base. The orientation is the same as in Figure 30A.

Figure 31C

- 15 Contact surface and V3 loop. The same as Figure 20B, but rotated around a horizontal axis to more clearly depict the 17b epitope.

Figure 31D

- 20 Electrostatic surface. The electrostatic potential is displayed at the solvent accessible surface, which is shaded according to the local electrostatic potential. The electrostatic shading is the same scale as that shown in Figure 30C. The surface that corresponds to the 17b epitope is the most electropositive region of the molecule. The V3 loop is truncated here, but  
25 sequence analysis shows that it is generally quite positively charged.

Figure 31E

- 30 Worm diagram of gp120. The gp120 is shown shaded according to the same scheme given in Figure 30A. The orientation is the same as in Figures 30C and 30D, that is, 90° from Figure 30A.

Figure 32

- 35 Schematic representation of the gp120 initiation of fusion. A single monomer of core gp120 is depicted in an orientation similar to Figures 29A and 29C. The "3"

-22-

symbolizes the 3-fold axis, from which gp41 interacts with the gp120 N- and C- termini to generate the functional oligomer. In the initial state of gp120 (on the surface of a virion), the V1/V2 loops are shown partially occluding the CD4 binding site. Following CD4 binding (now at a target cell, though above the glycocalyx), a conformational change is depicted as an inner/outer domain shift, with the dark circle denoting the formation of the Phe 43 cavity. This conformational change strains the interactions at the N- and C- termini of gp120 with the rest of the oligomer, priming the CD4-bound gp120 core. In the next step (which takes place directly adjacent to the target membrane), the chemokine receptor binds to the bridging sheet and the V3 loop (at the bottom left and right, respectively, of gp120), causing an orientational shift of core gp120 relative to the oligomer. This triggers further steps, which ultimately lead to the fusion of the viral and target membranes.

Figure 33

Structure of HIV-1 gp120 with neutralizing antibody and human receptor CD4.

**Figures for the Fourth Series of Experiments**

Figure 34A

Structure and orientation of the HIV-1 gp120 core.  $\alpha$  tracing of the gp120 core, which was crystallized in a ternary complex with two-domain sCD4 and Fab fragment of the 17b antibody(12), is shown. The gp120 core is seen from the perspective of CD4, and is oriented with the viral membrane at the top of the figure and the target cell membrane at the bottom. The N- and C-termini of the truncated gp120 core are labeled, as are the positions of structures related to the gp120 variable regions, V1-V5. The  $L_a$  and  $L_e$  surface loops(12) are

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shown. The position of the "Phe 43" cavity involved in CD4 binding is indicated by an asterisk. A gp120 surface implicated in binding to the CCR5 chemokine receptor (C. Rizzuto and J. Sodroski, submitted) is indicated. The perspectives in Figures 23B, C and D are indicated.

#### Figure 34B

View of the molecular surface of the gp120 outer domain, from the perspective indicated in Figure 34A. The molecular surface in the figure on the left is shaded according to the variability observed in gp120 residues among primate immunodeficiency viruses. The variability of the gp120 surface shown is underestimated since the V4 variable loop, which is not resolved in the structure, contributes to this surface. The position of the V5 region is shown. Also note the highly conserved glycosylation site (asparagine 356 and threonine/serine 358) within the L<sub>1</sub> loop, between the V5 and V4 regions. In the figure on the right, the V4 loop and the carbohydrates are modeled, as described in Materials and Methods.

#### Figure 34C

View of the gp120 molecular surface facing the target cell. Variability is indicated in the figure on the left, using the shading scheme as in Figure 34B. Note the clear demarcation between the conserved surface, which has been implicated in the formation of CD4i epitopes(18)and in chemokine receptor binding (C. Rizzuto and J. Sodroski, unpublished observations), and the variable surface of the outer domain. The recessed binding site for CD4 is indicated, flanked by the V1/V2 stem, which is labeled. The V4 loop and the carbohydrates are modeled in the figure on the right. The figure is shaded as indicated in Figure 34B particularly carbohydrates referred to elsewhere in this report are labeled.

#### Figure 34D

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View of the molecular surface of the gp120 core inner domain. In the figure on the left, variability is indicated by the shading scheme used in Figure 34B. The CD4-binding site is to the right of the figure, and the protruding V1/V2 stem is indicated. The conserved molecular surface, which is associated with the inner domain of the gp120 core, is devoid of known N-linked glycosylation. These are modeled in the figure on the right, which is shaded as described in Figure 23B.

10 Figure 35

The spatial relationship of epitopes on the HIV-1 gp120 glycoprotein.

Figure 35A

15 The molecular surface of the gp120 core is shown, from the same perspective as that in Figure 34A. The modeled N-terminal gp120 core residues, V4 loop and carbohydrate structures are included. The variability of the molecular surface is indicated, using the shading scheme described in Figure 34B. The approximate locations of the V2 and V3 variable loops are indicated. Note the well-conserved surfaces near the "Phe 43" cavity and the chemokine receptor-binding site (see Figure 34A).

Figure 35B

25 A  $\alpha$  tracing of the gp120 core, oriented similarly to Figure 34A. The gp120 residues within Figure 37A of the 17b CD4i antibody are shown. The residues implicated in the binding of CD4BS antibodies(20) are shown. Changes in these residues significantly affect the binding of at least 25 percent of the CD4BS antibodies listed in the table from the fourth series of experiments. The residues implicated in 2G12 binding(19) are shown. The V4 variable loop, which contributes to the 2G12 epitope, (19) is indicated by dotted lines (see figure 34A).

35 Figure 35C

The molecular surface of the gp120 core, oriented and shaded as in Figure 35B, is shown.

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Figure 35D

Approximate locations of the faces of the gp120 core, defined by the interaction of gp120 and antibodies. The molecular surface accessible to neutralizing ligands (CD4 and CD4BS, CD4i and 2G12 antibodies) is shown in white. The neutralizing face of the complete gp120 glycoprotein includes the V2 and V3 loops, which reside adjacent to the surface shown (see Figure 35A). The approximate location of the gp120 face that is poorly accessible on the assembled envelope glycoprotein trimer and therefore elicits only non-neutralizing antibodies(5, 6) is shown. The approximate location of an immunologically "silent" face of gp120, which roughly corresponds to the highly glycosylated outer domain surface, is also shown.

Figure 36

A likely arrangement of the HIV-1 gp120 glycoproteins in a trimeric complex. The gp120 core was organized into a trimeric array, based on the criteria discussed in the text. The perspective is from the target cell membrane, similar to that shown in Figure 34C. The CD4 binding pockets are indicated by black arrows, and the chemokine receptor-binding regions are darkly shaded. The lightly shaded areas indicate the more variable, glycosylated surface of the gp120 core. The approximate locations of the 2G12 epitopes are indicated by open arrows. The approximate locations for the V3 loops and V4 regions are shown. The positions of the V5 regions and some complex carbohydrate addition sites (asparaginase 276, 463, 356, 397 and 406) are shown. The approximate locations of the large V1/V2 loops, centered on the known positions of the V1/V2 stems, are indicated. On one of the gp120 subunits, the positions of the L<sub>D</sub> and L<sub>E</sub> loops are indicated. The distance of each of the gp120 monomers from the 3-fold symmetry axis is arbitrary.

Figures for the Fifth Series of Experiments

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Figure 37

The HIV gp120 derivative used in the binding assay. The wild-type gp120 and gp41 envelope glycoproteins are shown in the upper figure. Conserved (black) and variable (white) regions (25) are indicated. The wtΔ protein, which is derived from the primary macrophage-tropic YU2 HIV-1 isolate (7), is shown beneath the wild-type envelope glycoproteins. The N-terminal and V1/V2 deletions correspond to those previously described for the HXBc2 gp120 mutants Δ82 and Δ128-194, respectively (8,9). SIG=signal peptide.

Figure 38

The gp120-CCR5 binding assay.

Figure 38A

The radiolabeled wtΔ protein was incubated either with the parental L1.2 cells or with the L1.2-CCR5 cells. Incubations were carried out either in the absence or presence of sCD4 (100nM). The wtΔ protein bound to the cells is shown. The two bands represent different glycoforms of gp120.

Figure 38B

The wtΔ protein was incubated with both sCD4 and 17b antibody at the indicated concentrations prior to addition to the L1.2-CCR5 cells. The L1.2-CCR5 cells were incubated with 2D7 anti-CCR5 antibody or MIP-1β at the indicated concentrations prior to incubation with wtΔ-sCD4 complexes. The wtΔ protein bound to the cells is shown.

Figure 38C

The amount of radiolabeled wtΔ or selected mutant envelope glycoproteins precipitated by a mixture of HIV-1-infected patient sera (Total), precipitated by sCD4 and an anti-CD4 antibody (Bound(sCD4)), or bound to L1.2-CCR5 cells (Bound(CCR5)) is shown.

Figure 39

Structure of the HIV-1 gp120 region implicated in CCR5 binding.

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Figure 39A

A ribbon drawing of the HIV-1 gp120 glycoprotein (6) complexed with CD4 is shown. The perspective is that from the target cell membrane. The two amino-terminal domains of CD4 are shown. The gp120 inner domain is shown, the outer domain is shown and the "bridging sheet" is shown. The gp120 residues in which changes resulted in a  $\geq 90\%$  decrease in CCR5 binding are labeled. The V1/V2 stem and base of the V3 loop (strands  $\beta 12$  and  $\beta 13$  and the associated turn) are indicated.

Figure 39B

A molecular surface of the gp120 glycoprotein from the same perspective as that of Figure 39A is shown. Shaded surfaces are associated with gp120 residues in which changes resulted in either a  $\geq 75\%$  decrease, a  $\geq 90\%$  decrease or a  $\geq 50\%$  increase in CCR5 binding, when CD4 binding was at least 50% of that seen for the wt $\Delta$  protein.

Figure 39C

The surface depicted in Figure 39B is shaded according to the degree of conservation observed among primate immunodeficiency viruses (25).

Figure 39D

The molecular surface of the gp120 glycoprotein is shown, indicating residues in which changes resulted in a  $\geq 70\%$  decrease in 17b antibody binding, in the absence of sCD4.

Figure 39E

The molecular surface of the gp120 glycoprotein is shown, indicating residues in which changes resulted in a  $\geq 70\%$  decrease in CG10 antibody binding in the presence of sCD4. Residues in which changes significantly decreased CD4 binding (and thus indirectly decreased CG10 binding) are not shown. Images were made with Midas-Plus (Computer Graphics Lab, University of California, San Francisco) and GRASP (26).



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**Mimcs of CD4 With Enhanced Affinity For gp120**Figure 40

Illustration of the gp120-binding domain of CD4 and its interaction with the hydrophobic pocket of gp120.

5 Figure 41A

Active Halogen Reaction Scheme for modifying cysteine 43 mutants of CD4.

Figure 41B

10 Pyridyl Disulfide Reaction Scheme for modifying cysteine 43 mutants of CD4.

Figure 42

Some specific examples of cysteine 43 mutant derivatives produced with the active halogen reaction scheme.

Figure 43A

15 General reaction scheme for using a bifunctional reagent to modify the gp120-binding domain of CD4.

Figure 43B

20 Reaction scheme for using a bifunctional reagent to modify a residue in the gp120-binding domain of CD4 as applied to a cysteine residue.

Figure 44A and B

25 Use of 3-(2-pyridyldithio)propionic acid N-hydroxysuccinimide ester (SPDP), a bifunctional reagent, as an adaptor for modifying a residue in the gp120-binding domain of CD4.

Figure 45

Illustration of how modification can improve the fit between the gp120-binding domain of CD4 and the hydrophobic pocket in gp120.

30 Figure 46

Illustration of some of the residues lining the hydrophobic pocket of gp120. The residues lining the hydrophobic pocket of gp120 include: Trp (112), Leu (116), Pro (118), Phe (210), Val (255), Ser (375), Asn (377), Phe (382), Ile (424), Met (426), Trp (427), Asn (428), Ala (433), Gly (473), and Met (475)

35

Figure 47

-29-

Computer-generated ribbon drawing of the tertiary structure of CD4 and gp120 interacting. CD4 is toward the bottom and gp120 is toward the top.

Figure 48

- 5 Reaction scheme for chemically modifying tyrosine residues. R1 may be selected from the group shown in Figure 44. An alternative mechanism may be achieved as shown on page 365 of Structure and Protein Chemistry by Jack Kyte (1994), in which a diazonium salt participate  
10 in electrophilic aromatic substitution with tyrosine.

Figure 49

Schematic showing the structural domains of gp120.

**gp120 Variants as Vaccine For HIV Infection**

- 15 Figure 50

Depiction of the gp120 Oligomer.

Figure 51

Depiction of the pocket of gp120 formed after the binding of CD4 to gp120.

- 20 Figure 52

The topology for the gp120 ( $\Delta 82$ ,  $\Delta V1/2$ ,  $\Delta V3$ ,  $\Delta C5$ ) construct.

**Coordinates and Contacts**

- 25 Figure 53

- Shows the x-ray crystallography obtained atomic coordinate data of the gp120 ternary complex of HIV-1 GP120 complexed with CD4 and Fab 17b having space group P2221 and unit cell dimensions  $a=71.643$ ,  $b=88.130$ ,  
30  $c=196.7$ . The raw data and the coordinates were described in U.S. Serial No. 09/100,764, filed June 18, 1998 and U.S. Serial No. 08/967,708, filed November 10, 1997, on which this subject application claims priority. These documents are subjected for public inspection.  
35 The contents of these applications are incorporated into this application by reference. The coordinates have been deposited in the in the Brookhaven Protein Data

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Bank with the accession code Igcl. In addition, the coordinates may be obtained in the worldwide web: [www.pdb.bnl.gov](http://www.pdb.bnl.gov) after inputting "Igcl" for the above coordinates.

5 Figure 54

Provides a detailed list of all the contacts between gp120 (designated here as molecule A) and CD4 (designated here as molecule B).

Figure 55

- 10 Provides a detailed list of all the contacts between gp120 (designated here as molecule A) and the Fab 17b (the light chain is designated here as molecule C; the heavy chain is designated here as molecule D).

Detailed Description of the Invention

The invention relates to a crystals of gp120 suitable for x-ray diffraction. The three dimensional structure of gp120 provides information which has a number of  
5 uses; principally related to the development of pharmaceutical compositions which mimic the action of gp120. In an embodiment, the crystals comprising a portion of gp120. The portion of gp120 may contain the CD4 binding site. In another embodiment, the portion  
10 contains the chemokine receptor binding site. In a further embodiment, the portion of gp120 contains both the CD4 binding site and the chemokine receptor binding site.

15 In a separate embodiment, the portion of gp120 will be at least 100 amino acids long. In a preferred embodiment, the portion is at least 200 amino acid long.

The essence of the invention resides in the obtaining of  
20 crystals of gp120 of sufficient quality to determine the three dimensional (tertiary) structure of the protein by x-ray diffraction methods.

This invention provides crystals of sufficient quality  
25 to obtain a determination of the three-dimensional structure of gp120 to high resolution, preferably to the resolution of 2.5 angstroms.

The value of crystals of gp120 extends beyond merely  
30 being able to obtain a structure for gp120. The knowledge of the structure of gp120 provides a means of investigating the mechanism of action of these proteins in the body. For example, binding of these proteins to various receptor molecules can be predicted by various  
35 computer models. Upon discovering that such binding in fact takes place, knowledge of the protein structure then allows chemists to design and attempt to synthesize

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molecules which mimic the binding of gp120 to its receptors. This is the method of "rational" drug design.

5 One skilled in the art may use one of several methods to screen chemical entities for their ability to associate with gp120. This process may begin by visual inspection of, for example, the active site on the computer screen based on the gp120 coordinates. Docking may be  
10 accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

15 Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

20 GRID [P.J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem. 28:849-857 (1985)]. GRID is available from Oxford Universit, Oxford, UK.

25 MCSS [A. Miranker and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method", Proteins: Structure, Function and Genetics, 11:29-34 (1991)]. MCSS is available from Molecular Systems, Burlington, MA.

30 AUTODOCK [D.S. Goodsell and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins, Structure, Function, and Genetics, 195-202 (1990)] AUTODOCK is available from Scripps  
35 Research Institute, La Jolla, CA.

Once suitable entities or fragments have been selected,

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they can be assembled into a single compound or inhibitor. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of gp120. This would be followed by manual model building using software as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

CAVEAT [P.A. Bartell et al., "CAVEAT: A Program of Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc. 78, pp. 182-196 (1989)]. CAVEAT is available from the University of California, Berkeley, CA.

3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 35:2145-2154 (1992).

Instead of proceeding to build a gp120 inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other type of binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include:

LUDI [H.-J. Bohm "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6:61-78 (1992)]. LUDI is available from Biosym Technologies, San Diego, CA.

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LEGEND [Y. Nishibata and A. Itai, Tetrahedron, 47:8985 (1991)]. LENGEND is available from Molecular Simulations, Burlington, MA.

5 Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., N.C. Cohen et al, "Molecular Modeling Software and Methods for Medicinal Chemistry", J. Med. Chem., 33:883-894 (1990). See also, M.A. Navia and M.A. Murcko, "The Use  
10 of Structural Information in Drug Design", Current Opinions in Structural Biology, 2:202-210 (1992). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention.  
15 Numerous methods and techniques are known in the art for performing this step, any of which may be used. See, e.g., P.S. Farmer, Drug Design, Ariens, E.J., ed., Vol. 10, pp. 119-143 (Academic Press, New York 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; C.  
20 Verlinde, Structure, 2:577-587 (1994); and I.D. Kuntz, Science 257:1078-1082 (1992). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

25 Thus, using these computer evaluation systems, a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds is effectively eliminated.

30 Once identified by the modeling techniques, the gp120 or CD4 antagonist may be tested for bioactivity using standard techniques. For example, structure of the invention may be used in binding assays using  
35 conventional formats to screen inhibitors. Suitable assays for use herein include, but are not limited to, the enzyme-linked immunosorben assay (ELISA), or a

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fluorescence quench assay. Other assay formats may be used; these assay formats are not a limitation on the present invention.

5 In another aspect, the gp120 structure of the invention permit the design and identification of synthetic compounds and/or other molecules which have a shape complimentary to the conformation of the gp120 active  
10 the coordinates of the gp120 structure of the invention may be provided in machine readable form, the test compounds designed and/or screened and their conformations superimposed on the structure of the invention. Subsequently, suitable candidates identified  
15 as above may be screened for the desired gp120 inhibitory bioactivity, stability, and the like.

Once identified and screened for biological activity, these inhibitors may be used therapeutically or  
20 prophylactically to block gp120 activity.

Accordingly, this invention also provides material which is the basis for the rational design of drugs which mimic the action of gp120.

25 The subject invention provides a crystal suitable for X-ray diffraction comprising a polypeptide having an amino acid sequence of a portion of a Human Immunodeficiency Virus envelope glycoprotein gp120.

30 The subject invention also provides the above-described crystals, which effectively diffract X-rays for determination of the atomic coordinates of the polypeptide to a resolution of 4 angstroms or better  
35 than 4 angstroms.

The subject invention also provides the above-described



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crystals, which effectively diffract X-rays for determination of the atomic coordinates of the polypeptide to a resolution of 2.5 angstroms or better than 2.5 angstroms.

5

The subject invention also provides the above-described crystals, wherein the portion of gp120 comprises a CD4 binding site.

10

The subject invention further provides the above-described crystals, further comprising a compound bound to the CD4 site.

15

The subject invention also provides the above-described crystals, wherein the portion of gp120 comprises a chemokine receptor binding site.

20

The subject invention also provides the above-described crystals, further comprising a compound bound to the chemokine receptor binding site.

25

The subject invention also provides the above-described crystals, wherein the portion of gp120 comprises a CD4 binding site and a chemokine receptor binding site.

30

The subject invention also provides the above-described crystals, further comprising of a first compound bound to the CD4 binding site of the polypeptide and a second compound bound to the chemokine receptor binding site of the polypeptide.

35

The subject invention also provides the above-described crystals, wherein the first compound is the second compound.

The subject invention also provides the above-described crystals, wherein the crystal is arranged in a space

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group P222<sub>1</sub>, so as to form a unit cell of dimensions  
a=71.6 Å, b= 88.1 Å, c=196.7 Å, and which effectively  
diffracts x-rays for determination of the atomic  
coordinates of the gp120 to a resolution of 2.5 Å or  
5 better.

10 The subject invention also provides the above-described  
crystals, wherein the polypeptide is a variant of gp120  
lacking the V1, V2, V3, and C5 regions.

The subject invention also provides the above-described  
crystals, wherein the gp120 variant comprises a portion  
of the conserved stem of the V1/V2 stem-loop structure.

15 The subject invention also provides the above-described  
crystals, wherein the gp120 variant comprises a portion  
of the base of the V3 loop.

20 The subject invention also provides the above-described  
crystals, wherein the gp120 variant comprises a portion  
of the C5 region.

25 The subject invention also provides the above-described  
crystals, wherein the polypeptide is a variant of gp120  
with 5% by weight of the carbohydrate residues linked to  
the gp120 in substantially the same manner as they are  
linked to gp120 in unmodified gp120.

30 The subject invention also provides the above-described  
crystals, wherein the polypeptide is a variant of gp120  
with 15% by weight of the carbohydrate residues linked  
to the gp120 polypeptide in substantially the same  
manner as they are linked to gp120 in unmodified gp120.

35 The subject invention also provides the above-described  
crystals, further comprising a Fab, a CD4, a polypeptide  
having amino acid sequence of a portion of CD4, or a

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combination thereof, bound to the gp120.

5 The subject invention also provides the above-described crystals, wherein the Fab is produced from an antibody to a discontinuous epitope.

10 The subject invention also provides the above-described crystals, wherein the monoclonal antibody is designated 17b.

15 The subject invention additionally provides a method for producing a crystal suitable for X-ray diffraction comprising: (a) deglycosylating a polypeptide having amino acid sequence of a portion of a gp120 wherein said portion is produced by deleting or replacing part of the gp120 to reduce the surface loop flexibility; (b) contacting the polypeptide with a ligand so as to form a complex which exhibits restricted conformational mobility; and (c) obtaining crystal from the complex so  
20 formed to produce a crystal suitable for X-ray diffraction.

25 The subject invention also provides the above-described methods, wherein the V1, V2, or V3 loop of the gp120 contained in the polypeptide are partially truncated, deleted or replaced.

30 The subject invention also provides the above-described methods, wherein the polypeptide lacks the V1, V2, V3 and C5 loop of the gp120.

35 The subject invention also provides the above-described methods, wherein the polypeptide also lacks up to fifty N-terminal amino acids of the gp120 or up to fifty C-terminal amino acid of gp120.

The subject invention also provides the above-described

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methods, wherein the ligand is a Fab, a CD4, or a polypeptide having amino acid sequence of a portion of CD4.

5 The subject invention also provides the above-described methods, wherein the resulting polypeptide after the deglycosylation contains at least 5% of the carbohydrate.

10 The subject invention also provides the crystal produced by the above-described methods.

The subject invention also provides a method for identifying a compound capable of binding to a portion  
15 of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining a binding site on the portion of gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising the portion of gp120; and (b) determining  
20 whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the gp120.

The subject invention also provides a method for  
25 designing a compound capable of binding to a portion of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining a binding site on the portion of gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal  
30 comprising the portion of gp120; and (b) designing a compound to fit the binding site.

Structure-based drug design has been known and was previously described. See e.g., Bugg et al. (1993) Sci.  
35 Amer., December: 92-98; Giranda (1994) Structure, 2:695-698; Lam et al. (1994) Science 263:380-384; and Navia et al. (1994) Circulation 89(4):1557-1566.

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The subject invention also provides the above-described methods, wherein the fitting is determined by shape complementarity or by estimated interaction energy.

- 5     The subject invention also provides the above-described methods, wherein the atomic coordinates are set forth in Figure 53.

- 10    The subject invention also provides a pharmaceutical composition comprising the compound identified by the above-described methods and a pharmaceutically acceptable carrier.

- 15    For the purposes of this invention "pharmaceutically acceptable carriers" means any of the standard pharmaceutical carriers. Examples of suitable carriers are well known in the art and may include, but not limited to, any of the standard pharmaceutical carriers such as a phosphate buffered saline solutions, phosphate  
20    buffered saline containing Polysorb 80, water, emulsions such as oil/water emulsion, and various type of wetting agents. Other carriers may also include sterile solutions, tablets, coated tablets, and capsules.

- 25    Typically such carriers contain excipients such as starch, milk, sugar, certain types of clay, gelatin, stearic acid or salts thereof, magnesium or calcium stearate, talc, vegetable fats or oils, gums, glycols, or other known excipients. Such carriers may also include  
30    flavor and color additives or other ingredients. Compositions comprising such carriers are formulated by well known conventional methods.

- 35    The subject invention also provides the above-described methods, wherein the compound is not previously known.

The subject invention also provides the compounds

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identified by the above-described methods.

The subject invention also provides the compound designed by the above-described methods.

5

The subject invention also provides a composition comprising the above-described compounds and a suitable carrier.

10 This invention also provides a method of inhibiting the interaction of HIV-gp120 with CD4 which comprises administering to a mammal a compound, with the proviso that the compound is not CD4, capable of disrupting two or more of the contacts between gp120 and CD4 as set  
15 forth in Figure 54.

This invention also provides a method for identifying a compound capable of binding to the CD4 binding site of Human Immunodeficiency Virus envelope glycoprotein gp120  
20 comprising: (a) determining the CD4 binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of gp120 capable of binding to CD4; and (b) determining  
25 whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the CD4 binding site of the gp120.

The molecular interaction on HIV with CD4 is between the  
30 HIV envelope glycoprotein gp120 and the D1 domain of CD4. The crystal structure of the complex between the deglycosylated core of gp120 and the D1D2 fragment of human CD4 defines this interaction in atomic detail (Nature paper). Although there is an extensive  
35 interface between these components, the nexus of the interaction brings together those residues demonstrated by mutational analyses to those most crucial for

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binding. Phe 43 and Arg 59 from CD4 and Asp 368, Glu 370 and Trp 427 from gp120 (*Nature* paper, Fig. 3j). This dominant sub-site comprises gp120 residues 365-368, 370-371, 425-430 and 473. In addition, Phe 43 closes  
5 off a pocket on the HIV surface to form a large cavity ( $152\text{\AA}^3$ ) at this interface (*Nature* paper, Fig. 3b). Residues that line the Phe 43 pocket include Trp 112, Val 255, Thr 257, Glu 370, Phe 382, Tyr 384, Try 427, Met 475 and main-chain atoms of 256 and 375-377.

10

The atomic coordinates of the crystallographic model also define the binding surface to be exploited by high-affinity compounds that will have the property to inhibit the gp120-CD4 interaction, and thereby the  
15 attachment of HIV to CD4-positive cells. This definition of the surface provides practioners skilled in the art with the means to design such compounds. Appropriate fragments or chemicals entities for the design of such compounds can be formed through the use  
20 of specialized computer programs such as GRID, DOCK and LUDI. Computer graphical representatives of these entitles can then be composed into appropriate chemical compounds, using the crystal structure as a template. Medicinal chemists skilled in the art can then  
25 synthesize appropriate chemical compounds to implement these designs. Not all such compounds will bind and have inhibitory properties, but a sufficient portion will do so to provide the designed lead compounds for drug discovery. Such leads can then be developed by the  
30 methods of structure-based drug design using crystallized complexes between these compounds and deglycosylated core gp120.

A compound that will bind to the dominant sub-site of  
35 the CD4 intermolecular interface will have surface properties that are complementary to the surface properties of the sub-site itself. The surface of the

This invention also provides the above-described  
35 methods, wherein the fitting is determined by shape  
complementarity or by estimated interaction energy.



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This invention also provides the above-described methods, wherein the atomic coordinates are set forth in Figure 53.

5 This invention also provides a pharmaceutical composition comprising the compound identified the by above-described methods and a pharmaceutically acceptable carrier.

10 This invention also provides the above-described methods, wherein the compound is not previously known.

This invention also provides the compound identified by the above-described methods.

15

This invention also provides the compound designed by the above-described methods.

20 This invention also provides a composition comprising the above-described compounds and a suitable carrier.

This invention also provides a method of inhibiting Human Immunodeficiency Virus infection in a subject comprising administering effective of amount of the  
25 above-described composition to the subject.

In embodiments of the above-described methods, the above-described compounds are nonpeptidyl.

30 This invention provides a method for identifying a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the chemokine receptor binding site on the gp120 based on  
35 the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having the amino acid sequence of a portion of gp120 capable of

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binding to the chemokine receptor; and (b) determining whether a compound would fit into the binding site, a positive fit indicating that the compound is capable of binding to the chemokine receptor binding site of the gp120.

This invention also provides a method for designing a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising: (a) determining the chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having the amino acid sequence of a portion of gp120 capable of binding to the chemokine receptor; and (b) designing a compound to fit the chemokine receptor binding site.

This invention also provides the above-described methods, wherein the crystal further comprises a chemokine receptor, a second polypeptide having amino acid sequence of a portion of chemokine receptor, an antibody or a Fab capable of binding to the chemokine receptor binding site or a compound known to be capable of binding to the chemokine receptor binding site, bound to the polypeptide.

This invention also provides the above-described methods, wherein the fitting is determined by shape complementarity or by estimated interaction energy.

This invention also provides the above-described methods, wherein the atomic coordinates are set forth in Figure 53.

The pharmaceutical composition comprising the compound identified by the above-described methods and a pharmaceutically acceptable carrier.

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This invention also provides the above-described methods, wherein the compound is not previously known.

5 This invention provides compounds identified by the above-described methods. This invention provides compounds designed by above-described methods.

A composition comprising the above-described compounds and a suitable carrier.

10

Additionally, this invention provides a method of inhibiting Human Immunodeficiency Virus infection in a subject comprising administering effective of amount of the above-described composition to the subject, thereby  
15 inhibiting Human Immunodeficiency Virus infection.

20

This invention further provides a method of inhibiting the interaction of HIV-gp120 with chemokine receptor which comprises administering to a mammal a compound capable of disrupting two or more of the contacts between gp120 and chemokine receptor as set forth in Figure 55, thereby inhibiting the interaction of HIV-gp120 with chemokine receptor with the proviso that the compound is not a chemokine receptor. In an embodiment,  
25 the compound is nonpeptidyl.

**Table Summarizing the CCR5-binding residues of gp120**

	SET A	117, 121, or 123
	SET B	207
30	SET C	330
	SET D	419, 420, 421, 422, 437, 438, 440, 441, 442, or 444

This invention further provides a method of inhibiting cell entry by HIV, comprising blocking or inhibiting the  
35 residues from 2 or more the sets of the CCR5-binding residues set forth above, thereby inhibiting or preventing gp120 from binding to CCR5 and thereby

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inhibiting cell entry by HIV.

This invention also provides the above described method wherein 3 or more the sets of the CCR5-binding residues  
5 set forth above are blocked or inhibited from interacting with CCR5.

This invention also provides the above described methods, wherein the blocking or inhibiting comprises  
10 contacting the CCR5-binding residues with an antibody.

This invention also provides the above-described methods, wherein the compound is nonpeptidyl.

15 This invention provides a substance mimicking the human immunodeficiency virus envelope glycoprotein gp120-binding region of CD4 wherein the size of a residue or analog thereof, corresponding to the phenylalanine at position 43 in the native CD4, is larger than the size  
20 of phenylalanine so as to fill the pocket on gp120 which extends beyond position 43 in the gp120/CD4 complex and increase the affinity for gp120.

As used herein, residue or analog thereof includes amino  
25 acids (both individually and as part of a polypeptide chain), modified amino acids, amino acid analogs, and chemical compounds that can be substituted for the amino acids that ordinarily make up the CD4 polypeptide chain. (Also see the discussion of peptidomimetics, synthetic  
30 polypeptides, and polypeptide analogs below.)

This invention also provides the above-described substance, wherein the substance is a peptidomimetic analog, a synthetic polypeptide, a standard polypeptide,  
35 or a polypeptide analog.

As used herein, the substance mimicking the gp120-

binding domain of CD4 embraces a wide range of compounds. In addition to naturally-occurring forms of polypeptides derived from CD4, the present invention also embraces other CD4 polypeptides such as polypeptide  
5 analogs of CD4. Such analogs include fragments of CD4. Following the procedures of the published application by Alton et al. (WO 83/04053), one can readily design and manufacture genes coding for microbial expression of polypeptides having primary conformations which differ  
10 from that herein specified for in terms of the identity or location of one or more residues (e.g., substitutions, terminal and intermediate additions and deletions). Alternately, modifications of cDNA and genomic genes can be readily accomplished by well-known  
15 site-directed mutagenesis techniques and employed to generate analogs and derivatives of the CD4 polypeptide. Such products share at least one of the biological properties of CD4 but may differ in others.

20 As examples, products of the invention include those which are foreshortened by e.g., deletions; or those which are more stable to hydrolysis (and, therefore, may have more pronounced or longerlasting effects than naturally-occurring products); or which have been  
25 altered to delete or to add one or more potential sites for O-glycosylation and/or N-glycosylation or which have one or more cysteine residues deleted or replaced by e.g., alanine or serine residues and are potentially more easily isolated in active form from microbial  
30 systems; or which have one or more tyrosine residues replaced by phenylalanine and bind more or less readily to target proteins or to receptors on target cells. Also comprehended are polypeptide fragments duplicating only a part of the continuous amino acid sequence or  
35 secondary conformations within gp120, which fragments may possess one property of gp120 and not others. It is noteworthy that activity is not necessary for any one or

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more of the polypeptides of the invention to have therapeutic utility or utility in other contexts, such as in assays of gp120 antagonism. Competitive antagonists may be quite useful in, for example, cases  
5 of overproduction of gp120.

Of applicability to polypeptide analogs of the invention are reports of the immunological property of synthetic peptides which substantially duplicate the amino acid  
10 sequence extant in naturally-occurring proteins, glycoproteins and nucleoproteins. More specifically, relatively low molecular weight polypeptides have been shown to participate in immune reactions which are similar in duration and extent to the immune reactions  
15 of physiologically-significant proteins such as viral antigens, polypeptide hormones, and the like. Included among the immune reactions of such polypeptides is the provocation of the formation of specific antibodies in immunologically-active animals [Lerner et al., Cell, 23,  
20 309-310 (1981); Ross et al., Nature, 294, 654-658 (1981); Walter et al., Proc. Natl. Acad. Sci. USA, 78, 4882-4886 (1981); Wong et al., Proc. Natl. Sci. USA, 79, 5322-5326 (1982); Baron et al., Cell, 28, 395-404 (1982); Dressman et al., Nature, 295, 185-160 (1982);  
25 and Lerner, Scientific American, 248, 66-74 (1983). See also, Kaiser et al. [Science, 223, 249-255 (1984)] relating to biological and immunological properties of synthetic peptides which approximately share secondary structures of peptide hormones but may not share their  
30 primary structural conformation.

This invention also provides the above-described substances, wherein the modification increases the hydrophobicity or size of the residue or analog thereof  
35 at position 43.

This invention also provides the above-described

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substances, wherein the modification comprises directly or indirectly linking a hydrophobic compound to a residue or analog thereof at position 43 of the domain.

- 5 This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof that is bulkier than phenylalanine.
- 10 This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof larger than 7 Å across its longest dimension.
- 15 This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof larger than 10 Å across its longest dimension.
- 20 This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof larger than 15 Å across its longest dimension.
- 25 This invention provides the above described substance which enhances hydrophobic interactions to residues that line the pocket. In another embodiment, this invention provides the above described substance which enhances hydrogen bonding to residues that line the pocket.
- 30 a separate embodiment, this invention provides the above described substance which enhances electrostatic interactions with residues that line the pocket. In a still separate embodiment, this invention provides the above described substance which enhances surface fit
- 35 with residues that line the pocket.

This invention also provides the above-described

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substances, wherein the modification involves replacement of the residue at position 43 with a cysteine. This invention further provides that the substitution of the sulfhydryl group of this cysteine.

5

This invention also provides the above-described substances, wherein the modification involves replacement of the residue at position 43 with a tyrosine. This invention further provides that the substitution of this tyrosine

10

This invention also provides the above-described substances, wherein the modification comprises directly or indirectly linking an adaptor residue or analog thereof to position 43.

15

This invention also provides the above-described substances, wherein the adaptor residue or analog thereof is directly or indirectly linked to a hydrophobic compound, thus forming a complex.

20

This invention also provides the above-described substances, wherein the complex is bulkier than phenylalanine.

25

This invention also provides the above-described substances, wherein the complex is larger than 7 Å across its longest dimension.

30

This invention also provides the above-described substances, wherein the complex's longest dimension is longer than phenylalanine's longest dimension

35

This invention also provides the above-described substances, wherein the complex is larger than 10 Å across its longest dimension.



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substances, wherein the modification results in a residue or analog thereof, wherein the residue's longest dimension is longer than phenylalanine's longest dimension.

5

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof that contains a localization of negative charge so as to render the gp120-binding domain of CD4 able to hydrogen bond more strongly with the hydroxyl-containing side chains lining gp120.

10

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof that contains a localization of charge so as to render the gp120-binding domain of CD4 able to hydrogen bond more strongly with the hydroxyl-containing side chains lining gp120.

15

This invention also provides the above-described substances, wherein the modification results in a residue or analog thereof that contains at least one additional hydroxyl group.

20

Placing a tyrosine residue at position 43 is an example of a modification resulting in a residue that contains a hydroxyl group. Further, the oxygen of the hydroxyl group has a localization of negative charge so as to render the gp120-binding domain of CD4 able to hydrogen bond more strongly with the hydroxyl-containing side chains lining gp120. Further, the hydrogen of the hydroxyl group has a localization of charge so as to render the gp120-binding domain of CD4 able to hydrogen bond more strongly with the hydroxyl-containing side chains lining gp120.

25

30

35

This invention also provides the above-described

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This invention further provides a pharmaceutical composition capable of inhibiting cell entry by HIV, comprising (a) an effective amount of the above-described substance; and (b) a pharmaceutically acceptable carrier.

The actual effective amount will be based upon the size of the polypeptide, the biodegradability of the polypeptide, the bioactivity of the polypeptide and the bioavailability of the polypeptide. If the polypeptide does not degrade quickly, is bioavailable and highly active, a smaller amount will be required to be effective. The effective amount will be known to one of skill in the art; it will also be dependent upon the form of the polypeptide, the size of the polypeptide and the bioactivity of the polypeptide. Variants of CD4 with lower affinity for gp120 will require higher dosages than variants of CD4 with higher affinity for gp120. One of skill in the art could routinely perform empirical activity tests to determine the bioactivity in bioassays and thus determine the effective amount.

Pharmaceutically acceptable carriers are well known to those skilled in the art and have been described supra.

A pharmaceutical composition for treating or preventing HIV infection, comprising (a) an effective amount of the above-described substances; and (b) a pharmaceutically acceptable carrier.

This invention further provides a composition capable of inhibiting cell entry by HIV, comprising (a) an effective amount of the above-described substances; and (b) a suitable carrier.

This invention further provides a pharmaceutical composition for treating or preventing HIV infection,

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comprising (a) an effective amount of the above-described substances; and (b) a pharmaceutically acceptable carrier.

5 This invention further provides a composition for treating or preventing HIV infection, comprising (a) an effective amount of the above-described substances; and (b) a suitable carrier.

10 This invention further provides a method of inhibiting cell entry by HIV, comprising contacting the cells with an effective amount of the above-described substances, thereby inhibiting cell entry by HIV.

15 This invention further provides a method of treating or preventing HIV infection in a subject, comprising administering to the subject an effective amount of the above-described substances, thereby treating or preventing HIV infection.

20

The invention provides a variant of gp120 which presents a hidden, conserved, neutralization epitope. In an embodiment, the amino acid of the above variant at position 375 is changed from a Serine to a Trptophan.

25 In a further embodiment, the variant further comprise one of the following changes: 88N to P, 102E to L, 113D to R, 117K to W, 257T to A, 266A to E, 386N to Q, 395W to S, 421K to L, 470P to G, 475M to S, 485K to V or a combination thereof.

30

This invention further provides a composition comprising the above-described variant and a suitable carrier.

35 In a specific embodiment, "composition" as used herein means pharmaceutical compositions comprising therapeutically effective amounts of polypeptide

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products of the invention together with suitable diluents, preservatives, solubilizers, emulsifiers, adjuvants and/or carriers useful in therapy. A "therapeutically effective amount" as used herein refers to that amount which provides a therapeutic effect for a given condition and administration regimen. Such compositions are liquids or lyophilized or otherwise dried formulations and include diluents of various buffer content (e.g., Tris-HCl., acetate, phosphate), pH and ionic strength, additives such as albumin or gelatin to prevent absorption to surfaces, detergents (e.g., Tween 20, Tween 80, Pluronic F68, bile acid salts), solubilizing agents (e.g., glycerol, polyethylene glycerol), anti-oxidants (e.g., ascorbic acid, sodium metabisulfite), preservatives (e.g., Thimerosal, benzyl alcohol, parabens), bulking substances or tonicity modifiers (e.g., lactose, mannitol), covalent attachment of polymers such as polyethylene glycol to the protein, complexation with metal ions, or incorporation of the material into or onto particulate preparations of polymeric compounds such as polylactic acid, polglycolic acid, hydrogels, etc, or onto liposomes, microemulsions, micelles, unilamellar or multilamellar vesicles, erythrocyte ghosts, or spheroplasts. Such compositions will influence the physical state, solubility, stability, rate of in vivo release, and rate of in vivo clearance of the administered materials. The choice of compositions will depend on the physical and chemical properties of the protein having the biological activity. For example, a product derived from a membrane-bound form of the protein may require a formulation containing detergent. Controlled or sustained release compositions include formulation in lipophilic depots (e.g., fatty acids, waxes, oils). Also comprehended by the invention are particulate compositions coated with polymers (e.g., poloxamers or poloxamines) and the variants coupled to antibodies

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directed against tissue-specific receptors, ligands or antigens or coupled to ligands of tissue-specific receptors. Other embodiments of the compositions of the invention incorporate particulate forms protective  
5 coatings, protease inhibitors or permeation enhancers for various routes of administration, including parenteral, pulmonary, nasal and oral.

For the purposes of this invention "suitable carriers"  
10 means any of the standard carriers used in the pharmaceutical industry. Examples of suitable carriers are well known in the art and may include, but not limited to, any of the standard pharmaceutical carriers such as a phosphate buffered saline solutions, phosphate  
15 buffered saline containing Polysorb 80, water, emulsions such as oil/water emulsion, and various type of wetting agents. Other carriers may also include sterile solutions, tablets, coated tablets, and capsules.

20 Typically such carriers contain excipients such as starch, milk, sugar, certain types of clay, gelatin, stearic acid or salts thereof, magnesium or calcium stearate, talc, vegetable fats or oils, gums, glycols, or other known excipients. Such carriers may also include  
25 flavor and color additives or other ingredients. Compositions comprising such carriers are formulated by well known conventional methods.

This invention also provides a vaccine comprising the  
30 above-described variant. Such a vaccine may further comprise a suitable adjuvant.

Vaccines and adjuvants are well-known to those skilled in the art. Using a vaccine, comprising adjuvants or  
35 not, one may induce or stimulate the immune response of an individual. The immune response may vary, e.g. a humoral or cell-mediated immune response. Adjuvants are

chemical compounds that enhance the immunogenicity of the vaccine so as to enhance the stimulation and induction of the immune response.

5 In a specific embodiment, the vaccine is administered to a subject. As used herein, "subject" means any animal or artificially modified animal capable of becoming HIV-infected. Artificially modified animals include, but are not limited to, SCID mice with human immune systems.

10

In the preferred embodiment, the subject is a human. In another embodiment, the subject is a human infected with HIV.

15 As used herein, a "human infected with HIV" means an individual having at least one of his own cells infected by HIV. As used herein, an HIV-infected cell is a cell wherein HIV has been produced. A non-HIV-infected subject means a subject not having any cells infected by  
20 HIV. In one embodiment, a non-HIV-infected subject is an HIV-exposed subject. As used herein, an HIV-exposed subject is a subject who has HIV present in his body, but has not yet become HIV-infected. For example, a subject may become HIV-exposed upon receiving a needle  
25 stick injury with an HIV-contaminated needle.

In a specific embodiment of the invention, one may first crystals of gp120 of sufficient quality to determine the three dimensional (tertiary) structure of the protein by  
30 x-ray diffraction methods. The value of crystals of gp120 extends beyond merely being able to obtain a structure for gp120. The knowledge of the structure of gp120 provides a means of investigating the mechanism of action of these proteins in the body. For example,  
35 binding of these proteins to various receptor molecules can be predicted by various computer models. Upon discovering that such binding in fact takes place,

knowledge of the protein structure then allows chemists to design and attempt to synthesize molecules which mimic the binding of gp120 to its receptors. This is the method of "rational" drug design. Using such methods, one may determine a variant of gp120 which presents a hidden, conserved, neutralization epitope.

This invention further provides an antibody induced by the above-described vaccine. Specifically, the antibody may be a polyclonal antibody or a monoclonal antibody.

An antibody comprises intact immunoglobulin molecules, substantially intact immunoglobulin molecules and those portions of an immunoglobulin molecule that contains the paratope, including those portions known in the art as Fab, Fab', F(ab')<sub>2</sub> and F(v), which portions are preferred for use in the therapeutic methods described herein. In another embodiment, the antibody is a single-chain antibody.

As used herein, "polyclonal antibodies" may comprise different sera whereas "monoclonal antibody" comprises antibodies, each of which will recognize one single epitope. Methods for production of monoclonal antibodies are well-known in the art.

In order to determine variants of gp120 which presents a hidden, conserved, neutralization epitope, the gp120 structure of the invention permit the design and identification of synthetic compounds and/or other molecules which have a shape complimentary to the conformation of the gp120 active site of the invention. Using known computer systems, the coordinates of the gp120 structure of the invention may be provided in machine readable form, the test compounds designed and/or screened and their conformations superimposed on the structure of the invention. Subsequently, suitable

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candidates identified as above may be screened for the desired gp120 inhibitory bioactivity, stability, and the like.

5 Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block gp120 activity. Such compounds may prove useful as vaccines.

10 This invention provides a vaccine comprising a polypeptide having 6 or more amino acids in the same spatial proximity to each other as the amino acids from the Phe 43 cavity of naturally occurring gp120.

15 This invention also provides the above-described vaccine, wherein the 6 or more amino acids are identical to the amino acids of naturally occurring gp120.

20 This invention further provides the above-described vaccines, wherein the amino acids are within 1 angstrom of their distances in naturally occurring gp120.

This invention also provides the above-described vaccines, wherein the amino acids are within 3 angstroms of their distances in naturally occurring gp120.

25 This invention provides the above-described vaccines, wherein the amino acids are within 5 angstroms of their distances in naturally occurring gp120.

30 This invention also provides the above-described vaccines, wherein the polypeptide is or is part of a conserved neutralization epitope.

35 This invention further provides the above-described vaccines, further comprising a carrier.

This invention also provides the above-described



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vaccines, further comprising an adjuvant.

5 This invention provides a vaccine comprising a polypeptide having 6 or more continuous amino acids from the Phe 43 cavity of gp120.

10 This invention provides the above-described vaccines, wherein the polypeptide is or is part of an epitope a conserved neutralization epitope.

15 This invention also provides the above-described vaccines, further comprising a carrier.

20 This invention further provides the above-described vaccines, further comprising an adjuvant.

25 This invention further provides a vaccine comprising a polypeptide having 6 or more amino acids in the same spatial proximity to each other as the surface accessible amino acids adjacent to the Phe 43 cavity of naturally occurring gp120.

30 This invention also provides the above-described vaccines, wherein the 6 or more amino acids are identical to the amino acids of naturally occurring gp120.

35 This invention provides the above-described vaccines, wherein the amino acids are within 1 angstrom of their distances in naturally occurring gp120.

This invention also provides the above-described vaccines, wherein the amino acids are within 3 angstroms of their distances in naturally occurring gp120.

This invention further provides the above-described vaccines, wherein the amino acids are within 5 angstroms

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of their distances in naturally occurring gp120.

5 This invention also provides the above-described vaccines, wherein the polypeptide is or is part of a conserved neutralization epitope.

This invention further provides the above-described vaccines, further comprising a carrier.

10 This invention also provides the above-described vaccines, further comprising an adjuvant.

15 This invention also provides the above-described vaccines, wherein the surface accessible amino acids comprise Lysine 432, Proline 369, and Threonine 373.

20 This invention further provides a vaccine comprising a polypeptide having 6 or more continuous surface accessible amino acids adjacent to the Phe 43 cavity of gp120.

25 This invention also provides the above-described vaccines, wherein the polypeptide is or is part of a conserved neutralization epitope.

30 This invention further provides the above-described vaccines, further comprising a carrier. This invention also provides the above-described vaccines, further comprising an adjuvant.

35 Many animal viruses target specific host cells for infection by attachment to cell surface receptor molecules unique to these cells. These viral receptors have particular roles in the normal functioning of these cells. The virus simply subverts these functions in order to effect entry into the cell. Certain molecules on the viral surface can in turn be the target of

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antibodies raised by the host in defense against this parasitic attack. Viruses can evade such antibody immunity by mutating their surface proteins. The receptor binding site, however, must remain constant.

5 It therefore evolves to be protected from antibody surveillance.

Application to HIV vaccine:

- 10 The viral surface protein, gp120 (which appears to be a trimer on the surface of the virion), plays a central role in immune evasion. The precise mechanism of gp120 immune evasion thus far remains unknown, but the structure of the gp120 - CD4 - Fab 17b complex reveals
- 15 several crucial features:
1. The CD4 binding site is very large (larger than the typical antibody footprint).
  2. The V1/2 variable loop is oriented to mask the CD4 binding site.
  - 20 3. The V3 variable loop is not near the CD4 binding site (on a monomer), but the tip of this loop could interact with Fab 17b, which marks the second receptor binding site.
  4. The CD4 binding site undergoes conformational
  - 25 changes upon CD4 binding.

From the structure, the following details of the mechanism of gp120 immune evasion become clear:

1. The V1/2 loop occludes the CD4 binding site and
- 30 allow CD4 binding. With most viruses, which bind to rare cellular receptors, such a mechanism of immune evasion would not work; the virus would not find the proper receptor at high enough frequency to ensure viral propagation. It is the clustering
- 35 of CD4 positive cells in such places as the thymus which allows this mechanism to function in the particular case of HIV.

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2. The virus masks constant regions involved in both CD4 and second receptor binding; the act of CD4 binding induces conformational changes in gp120 which unmask these regions.
- 5 3. The V3 loop, which forms part of the conserved second receptor binding site, is one of the regions unmasked by CD4 binding.

10 This invention uses an antigen which mimics the conformation of gp120 on the surface of the HIV-virion, with deletions in the variable loop regions to expose the conserved CD4 binding site. It is already known that CD4-binding site antibodies are widely neutralizing, and moreover, are found in virtually all  
15 patients (although they tend to only be found late in the course of infection -- the initial antibodies produced early in the course of infection have the V1/2 or V3 loop as epitopes).

20 This invention provides a vaccine composed of a stabilized oligomer of gp120, with truncations in the variable loop regions to expose the conserved CD4 binding site, would elicit widely neutralizing antibodies against HIV.

25

Details: Oligomer stabilization (Figure 50):

1. Appropriately placed cysteine mutations, which would then form stabilizing disulfide bonds.
2. Linkers between consecutive N- and C- termini.  
30 (The structure shows that the N- and C- termini of gp120 are relatively close together. A genetically constructed flexible linker of amino acids between the C- terminus of one monomer and the N- terminus of an adjacent monomer would also serve to  
35 covalently stabilize the oligomer.)
3. A gp140 construct (the extracellular portion of gp120 + gp41) with a mutation at the gp120/gp41

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consensus cut site.

4. Trimers of GCN4 have been shown to enhance oligomerization. These oligomerization stabilizers could be added to the C-terminal tail of gp120.

5

Loop deletions:

Replacement of V1/2 loop with tripeptide Gly-Ala-Gly to expose of the CD4 binding site. Replacement of the V3 loop as well.

10

Stabilization of kinetically hidden epitopes of gp120. This invention uses gp120 which has been stabilized to elicit an immune response. gp120 may undergo conformational changes. However, only very few expose a conserved, neutralization epitope. This invention aims at using the information from the structure of gp120 to stabilize the hidden neutralization epitope of gp120. Specifically, the epitope may be stabilized by mutating the gp120 or alternatively, some epitope may be stabilized by ligand/drug interaction.

15

20

Specific examples are illustrated below:

**Example 1:**

The pocket of gp120 (Figure 51) only forms upon CD4 binding. If the residues along the pocket are mutated and was filled up, making it "stuck" in the CD4 conformation even without the binding CD4. Such mutation may include changing the Ser375 to Trp375, Val255 to Phe255 and Thr257 to Trp257.

30

The residues which lines the pocket include:

Trp 112 Leu 116 Pro 118 Phe 210 Val 255 Thr 257 Ser 375  
Asn 377 Phe 382 Ile 424 Met 426 Trp 427 Asn 428 Ala 433  
Gly 473 Met 475

35

**Example 2:**

Making disulfide bridges which tie protein domains. The

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Topology for gp120 ( $\Delta 82$ ,  $\Delta V1/2$ ,  $\Delta V3$ ,  $\Delta C5$ ) is shown in Figure 52. One can see the two domains, the N/C termini including  $\alpha 1$ , and a barrel around  $\alpha 2$ . A disulfide formed between  $\beta 2$  and  $\beta 21$  will tie the protein domains.

5 As another example, disulfide bridge may be formed between  $\beta 5$  and  $\beta 6$  connection and top of the barrel (e.g.  $\beta 10$ ).

**Example 3**

10 Cavities internal to the gp120 may be determined after knowing the three-dimensional structure of gp120. Analysis of all atoms are within 4 Angstroms of the surface defining each cavity allows mutations to be designed to determine if any large substitutions are

15 allowed. Below shows some example of the analysis:  
Val225 to Trp - not as good as 375 (below) -modeling shows some clashes with Met 475, although 475 should be able to move.

Ser375 to Trp - good fit (Note:the ser 375 mutation is incompatible with the Val225 mutation so only one can be

20 made at a time).

Following are the antibody binding results:

Table: Binding of the gp120 Variants to CD4BS Antibodies

Mutants	F105	<u>CD4BS antibodies</u>			
		15e	IgGbl2	21h	F91
255V/W	0.0	0.06	0.51	0.80	0.76
375S/W	0.0	0.36	0.05	0.72	0.0

30 Wild-type phenotype is 1.00 and decreases in recognition of below 1.

Control for CD4 and 17b Binding

Mutants	CD4	17b
255V/W	0.7	0.8
35 375S/W	0.9	1.0

The above result shows clearly that the mutations of Val255 to Trp, and Ser375 to Trp cause decrease of

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binding to CD4BS antibodies.

5 The cavity filling mutant 375S/W clearly exhibits reduction in binding of CD4-BS antibody binding. While the data look good, two of the CD4-BS antibodies (15e and 21 h) still bind with reasonable affinity.

10 The basic idea behind the cavity filling mutants is to stabilize the CD4-bound conformation of gp120 at the expense of the CD4-free conformation. Additional substitutions may then be made in combination with the 375S/W. For example, taking the known mutations which exhibit similar phenotypes to 375S/W (See Thali et al (1995), J.Virol. 67, 3978-3988).

15 88N/P: Since this substitution is very far from the CD4 interacting surface, the only way to explain the results is they affect the C1/C5 terminal regions which in some manner affect the relative stability of the gp120 conformations.

25 102E/L: This glutamic acid is on the surface of gp120 and appears to stabilize the alpha1/alpha5 helix interaction. However, the stabilization is weak. The only way to explain the observed phenotype is that in the CD4-minus conformation, the glutamic acid is somehow involved in a stabilizing interaction, perhaps to the nearby Arg that in this conformation is just out of reach.

30 113D/R: The aspartic acid stabilizes the bridging sheet residues Gln428 and Lys429, which are important for maintaining the CD4-bound conformation of gp120.

35 117K/W: The lysine helps stabilize the bridging sheet conformation, but this substitutions may also affects CCR5 binding so it may not be so good a choice.

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257T/A: Since this Thr is basically buried in the CD4-bound conformation, and indeed provides stabilizing hydrogen bonds, the only way to explain the phenotype of the T/A substitution is that Thr257 must be a critical element in maintaining the CD4-minus conformation. The residue is quite close 375W, so there may be some complications. If one places 375W in its preferred rotamer conformation, it clashes with Thr257-the mutation is accommodated by a slight change in rotamer conformation or by movement of the 375 backbone). So the T/A may actually help to accommodate the 375W change.

266A/E: The alanine is buried in the interface between the inner and outer domain. The substitution (on the face away from CD4 binding) most certainly effects thins conformationally, but since it is disruptive it is difficult to interpret.

386N/Q: This substitution is on the outer face of the outer domain and may not affect conformation. However, it does effect 21h the epitope of which is closer tot he inner domain so perhaps the loss of carbohydrate has long-range conformation effects.

395W/S: This substitution is also on the outer face of the outer domain. But it affects all the CD4-BS antibodies while retaining good CD4 binding.

421K/L: This is on bridging sheet. In the CD4-bound conformation, the Leu may pack nicely against Ileu423. Although this substitution may reduce CCR5 binding, the fact that it is far from where CD4 binds suggest that its effects may be conformational. (The effect 421K/D on CCR5 binding may be primarily electrostatic.)

470P/G and 475M/S: Both of these are close to the CD4-



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binding region, although both are buried and do not interact directly with CD4. Both retain good CD4 binding so the effect may be conformational.

- 5     485K/V: This is at the inner/outer domain interface. There may be steric clashes of the valine (the base of the Lys is buried) which may be disruptive.

10     This invention further provides vaccine design based upon conformational stabilization using the three-dimensional structure. See e.g. Malakauskas and Mayo Nature Structure Vol.5, p.470-475, entitled "Design, Structure and Stability of a hyperthermophilic protein variant," the content of which is incorporated into  
15     this application by reference.

20     The invention will be better understood by reference to the Experimental Details which follow, but those skilled in the art will readily appreciate that the specific experiments detailed are only illustrative, and are not meant to limit the invention as described herein, which is defined by the claims which follow thereafter.

FIRST SERIES OF EXPERIMENTS

5      Probability analysis of variational crystallization and its application to gp120, the exterior envelope glycoprotein of type 1 human immunodeficiency virus (HIV-1)

Summary

10      The extensive glycosylation and conformational mobility of gp120, the envelope glycoprotein of type 1 human immunodeficiency virus (HIV-1), pose formidable barriers for crystallization. To surmount these difficulties, we used probability analysis to determine the most  
15      effective crystallization approach and derive equations which show that a strategy, which we term variational crystallization, substantially enhances the overall probability of crystallization for gp120. Variational crystallization focuses on protein modification as  
20      opposed to crystallization screening. Multiple variants of gp120 were analyzed with an iterative cycle involving a limited set of crystallization conditions and biochemical feedback on protease sensitivity, glycosylation status, and monoclonal antibody binding.  
25      Sources of likely conformational heterogeneity such as N-linked carbohydrates, flexible or mobile N- and C-termini, and variable internal loops were reduced or eliminated, and ligands such as CD4 and antigen-binding fragments (Fabs) of monoclonal antibodies were used to  
30      restrict conformational mobility as well as to alter the crystallization surface. Through successive cycles of manipulation involving 18 different variants, we succeeded in growing six different types of gp120 crystals. One of these, a ternary complex composed of  
35      gp120, its receptor CD4, and the Fab of the human neutralizing monoclonal antibody 17b, diffracts to a minimum Bragg spacing of at least 2.2 Å and is suitable

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for structural analysis.

### Introduction

5 In conventional crystallizations of biological  
macromolecules, the protein or other macromolecular  
subject is treated as a fixed entity to be tested in a  
multitude of crystallization conditions. Despite  
advances such as sophisticated screening procedures(1,2)  
10 and crystallization robots(3,4), this approach often  
fails for components from complex biological systems.  
One of these, the subject of this study, is the HIV-1  
exterior envelope glycoprotein, gp120. In such cases,  
success may follow if the protein itself is varied.  
15 There are, however, many options in this vein and it is  
not clear how they might be prioritized. By way of  
background for this study, we first consider various  
options for the crystallization of conformationally  
complex macromolecules and then describe the  
20 characteristics of gp120.

**Crystallization by variation and modification.** For the  
more difficult crystallization challenges, which can be  
defined as those for which conventional screening fails,  
25 one typically tries to vary or modify the protein while  
maintaining biologically important properties.  
Meaningful results obtain since the integrity of  
internal structure and functional properties can often  
tolerate variation at the molecular surface where  
30 lattice contacts are made. The probability for success  
in crystallization is enhanced because flexible or  
heterogeneous surface features may be removed or because  
of the fortuitous introduction of lattice interactions.  
A prescient example that pre-dates the powerful methods  
35 of modern molecular biology was John Kendrew's screening  
of myoglobins from many different organisms until he  
found one, from sperm whale, that crystallized well(5).

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Indeed, human myoglobin requires a Lys to Arg substitution in order to produce crystals suitable for structural analysis(6). Conversely, crambin forms exceptionally well-ordered crystals despite being a mixture of two isoforms with sequence variation at internal residues(7).

There are many notable examples of variation or modification in the crystallization of macromolecules. Systematic variation in the species of origin, as pioneered with myoglobin(5), was also instrumental in the crystallization of the transcription initiating TATA-binding protein(8). Proteolysis is often used to define crystallizable fragments, following the early examples from enzymatic digestions of antibodies that produced crystallizable fragments (reviewed in (9)) and the bromelain release of hemagglutinin from the influenza virus membrane(10). Variation of recombinant constructs, often inspired by proteolytic definition, is now commonplace with the widespread use of molecular biology tools. Systematic variation in the length of DNA oligomers has proved essential in the structural studies of protein - nucleic acid complexes. The work of Jordan and Pabo on  $\lambda$  repressor(11) sets the example for transcription factors, and the principle extends to other complexes as for the nucleosome(12). The use of protein ligands to stabilize another protein of interest for crystallization has also been effective as in the study of actin through its complex with DNase I(13) and more generally through complexes with antigen-binding Fab fragments of antibodies (reviewed in (14)). The principle that the detergent solubilized lipid interface of membrane proteins is generally unavailable for lattice contacts has led to the concept that crystallizability will be enhanced if the non-variable surface area is increased, and this was demonstrated in practice in the crystallization of a bacterial

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cytochrome oxidase in complex with an antibody Fv fragment(15). Similarly, the anticipated conformational and compositional heterogeneity in carbohydrate moieties of glycoconjugates is expected to interfere with  
5 crystallization, and deglycosylation has proved essential for heavily glycosylated proteins such as human chorionic gonadotropin(16).

Characteristics of HIV gp120. HIV-1 induces acquired  
10 immunodeficiency syndrome (AIDS) in humans(17,18). The gp120 glycoprotein helps to mediate virus entry into cells through sequential recognition of two cellular receptors, the surface glycoprotein CD4(19,20) and a chemokine receptor (primarily CXCR4 or CCR5, depending  
15 on viral strain)(21-26). These high affinity interactions are attractive targets for mimetic drug design. Although the structure of the gp120-binding domain of CD4 and the identity of residues critical to its interaction with gp120 have been known for several  
20 years(27,28), this has not been sufficient for design of potent antagonists(29-31). As the major virus-specific antigen accessible to neutralizing antibodies, knowledge of the gp120 structure could also impact considerably on vaccine design. Despite this interest and considerable  
25 effort for several years with pure soluble protein, available in quantities as a byproduct in part from vaccine trials, gp120 has resisted crystallographic analysis.

30 The mature gp120 glycoproteins of different HIV-1 strains typically have 470-490 amino acid residues(32). Extensive N-linked glycosylation at 20-25 sites accounts for roughly half of the gp120 mass(32,33). Sequences from many different viral isolates show that gp120 has  
35 five variable regions (V1-V5) interspersed between relatively conserved regions (C1-C5)(32,34) and nine conserved disulfide bridges(33). Except for limited N-

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and C-terminal cleavage, proteolytic digestion does not reveal a sub-domain structure. Indeed, even after extensive proteolytic cleavage, the unreduced protein runs near its native molecular weight on SDS-PAGE (PDK, unpublished data).

The gp120 glycoprotein likely exhibits conformational flexibility. Some of the variable regions, the V2 and V3 loops in particular, are known to be exposed on the surface of the native protein and probably assume multiple conformations. The potential of gp120 to undergo conformational change is also evidenced by shedding, the CD4-induced dissociation of gp120 from the surface of the virus, by ligand-induced variations in monoclonal antibody binding(35,36), and by complex CD4-gp120 binding kinetics(37). These changes may be related to the functional role of gp120 in virus entry.

The extensive glycosylation and conformational heterogeneity of gp120 suggested that merely screening the protein through ever more exotic crystallization conditions would not produce well-diffracting crystals. We have analyzed the effectiveness of optimizing different crystallization factors given the specific characteristics of gp120. This led us to a strategy employing radical modification of the protein surface, primarily to reduce heterogeneity but also to create new potential lattice contacts. We derive equations which show that this strategy, which we term variational crystallization, substantially enhances the overall probability of crystallization for gp120. An iterative process, involving both biochemical and molecular biological techniques, was used to detect and remove chemical and conformational heterogeneity. In addition, protein ligands, namely CD4 and the Fab fragments of several monoclonal antibodies, were used to restrict conformational mobility. Progressive trials of 18

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different gp120 crystallization variants yielded six different crystals, at least one of which is suitable for structural analysis. This paradigm of crystallization, with a focus on protein modification rather than on crystallization screening, may aid in the structural analysis of other conformationally complex proteins.

#### Theoretical Analysis

10

Much of the crystallization literature is anecdotal, reflective perhaps of the diverse nature of proteins. Systematic quantitative studies have necessarily focused on robust, well characterized systems(38). If a particular protein fails to crystallize, one is faced with a bewildering array of options based on the experience with other often quite different proteins. In the absence of a comprehensive crystallization theory it is difficult to know how to proceed. Here, we devise an approximate theoretical underpinning for such decisions based on the ratio comparing crystallization probabilities before ( $P_i$ ) and after ( $P_f$ ) a modifying procedure. We define the enhancement in crystallization probability as  $\mathcal{E} = P_f / P_i - 1$  whereby  $\mathcal{E} = 0$  for no change and can reach a maximum,  $\mathcal{E}_{\max} = 1 / P_i - 1$ , that depends on the inverse of the initial probability.

In evaluating different crystallization strategies, one important consideration is effectiveness. Many factors affect crystallization, and a suitable crystallization approach depends on identifying and dealing with those that are most limiting. For example, if a protein were only 30% pure, the crystallization probability associated with such protein purity would be low and a purification strategy would be key; if a protein were 98% pure, further purification would most likely have

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little impact on the overall probability of crystallization. Factors that might be expected to affect the crystallization of gp120 are listed in Table 1, along with estimates of the effect of optimizing each factor given the specific characteristics of gp120.

Although identification of limiting crystallization factors can establish rough guidelines as to the appropriateness of a particular crystallization strategy, a better way to evaluate effectiveness (or perhaps to judge the progress of a specific crystallization effort) is by quantitative assessment of the enhancement in crystallization probability. For example, if 80% of all crystallizable proteins crystallize from a core set of 50 conditions(2), a strategy that involves screening ever larger arrays of crystallization conditions could at most enhance the probability of crystallization by only 25% over that for the first 50 conditions; further screening would yield increasingly diminishing returns. With this screening example, the quantitative enhancement of probability is straightforward to calculate, but it is not immediately apparent for the strategy of variational crystallization, which focuses on protein modification. We can consider two kinds of such modifications -- those designed to reduce heterogeneity and those related to expanding the number of crystallization candidates.

**Enhancement of surface homogeneity.** Crystalline order is explicitly dependent on lattice homogeneity. Reducing heterogeneity can be thought of as increasing the proportion of surface area available for formation of lattice contacts, increasing the probability of crystallization. The probability that a single lattice contact between two molecules may form is in part related to the fraction of surface area that is homogeneous on one molecule multiplied by the fraction



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homogeneous on the other, i.e.,

$$P(\text{homogeneous contact}) \propto H(\text{molecule 1}) \times H(\text{molecule 2}) \quad (1)$$

5 where H is defined as the homogeneous fraction of the surface. Consider the case where the molecule in question is the smallest repeating unit in a crystal, that is, the asymmetric unit. In such a case molecule 1 and molecule 2 are equal, and the above equation  
10 reduces to (% homogeneous surface)<sup>2</sup>. Now consider the same scenario with two lattice contacts; the probability that both are homogeneous is related to  $[(H - \partial_1)^2 \times (H - \partial_2)^2]$  where "H" is the homogeneous fraction of the surface which may form lattice contacts and " $\partial_n$ " is a  
15 function of the relative size and total number of lattice contacts other than contact n and the degree and distribution of surface homogeneity -- related to the occlusion of available surface area upon formation of each lattice contact as well as the spatial distribution  
20 of homogeneous surface over the molecular surface. Generalizing to case of "C" lattice contacts, the probability associated with homogeneous lattice formation is related to:

25

C

$$P(\text{lattice}) \propto [(H - \partial_1)^2 \times (H - \partial_2)^2 \times \dots \times (H - \partial_C)^2] = \prod_{n=1}^C (H - \partial_n)^2 \quad (2)$$

30 In the restricted case of one molecule per asymmetric unit, the observed average value of "C" ( $C_{ave}$ ) is ~4.5(39), with a minimum theoretical value for the most common space groups of 2 or 3(39). Since C may be relatively small, lattice contacts may make up only a  
35 small proportion of a macromolecule surface, with considerable surface heterogeneity tolerated. Thus, for example, many proteins that pack into well-ordered

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crystal lattices have disordered regions, with N- and C-termini as well as internal loops being unresolved.

5 Given a reduction in surface heterogeneity, what is the change in crystallization probability? Surface area is correlated with molecular mass (M) by the power law: surface area =  $6.3 \times M^{0.73}$ , which on average predicts surface area to within 4% for monomeric proteins (40). The fraction of homogeneous surface can thus be  
10 approximated as a ratio of molecular masses of the total and of the homogeneous portion of the protein:

$$H \approx [M(\text{homogeneous}) / M(\text{total})]^{0.73} \quad (3)$$

15 From Eqs. 2 and 3, it is now possible to estimate the enhancement in probability for crystallization upon reduction of heterogeneity. With the simplifying approximation  $\partial \bar{n} \approx 0$ , the probability ratio of before ( $P_i$ ) and after ( $P_f$ ) becomes

20

$$P_f / P_i \approx [(M(\text{homogeneous})_f / M(\text{total})_f)^{1.46 \times C} / [(M(\text{homogeneous})_i / M(\text{total})_i)^{1.46 \times C}] \quad (4)$$

25 Equation 4 is still not very useful, however, since  $M(\text{homogeneous})$  is unknown and molecule-specific. In reducing heterogeneity, however, it seems reasonable to assume that the removed portion, if it were a highly branched carbohydrate or a proteolytically exposed  
30 region, is completely heterogeneous. In such cases,  $[M(\text{homogeneous})_f \approx M(\text{homogeneous})_i]$  whether or not all heterogeneity has been removed. Assuming that  $C \approx C_{\text{ave}}$ , the enhancement ( $\mathcal{E}$ ) in probability on removal of a heterogeneous portion becomes

35

$$\mathcal{E}_r = P_f / P_i - 1 \approx [M(\text{total})_i / M(\text{total})_f]^{1.46 \times C_{\text{ave}}} - 1 \quad (5)$$

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This last equation allows the change in crystallization probability upon heterogeneity removal to be quantified. For example, consider a situation where a recombinant DNA approach is used to produce a protein with an affinity tag of 10 amino acid residues. Is it important to remove these presumably flexible residues? From Eq. 5, the answer depends on the protein size. For a 100-residue protein, removal of the tag would greatly enhance the crystallization probability by:  $\mathcal{E}_r = P_f / p_i$   
 $-1 = [110/(110-10)]^{1.46 \times 4.5} - 1 = 0.87$ , or almost 90%, whereas for a 500-residue protein the enhancement would be minimal,  $\mathcal{E}_r = 0.14$ .

Another variant of Equation 4 can be used to estimate the impact of adding a ligand of fixed structure to a molecule that contains heterogeneous portions. This expands the surface available for lattice contacts and effectively dilutes the heterogeneous component. It may be an approach of choice when the heterogeneity is essentially unremovable, such as at the lipid interface of detergent solubilized membrane proteins. One faces the difficulty of estimating the extent of heterogeneity to use Eq. 4, but this might be done by summing the residual variable components in gp120 or by topographical estimates for a membrane protein. (For example, for a sphere embedded symmetrically in a membrane of thickness  $h$ ,  $1-H = \text{area(heterogeneous)}/\text{area(total)} = h/[6Mv/(\pi N_o)]^{1/3}$ , where  $M$  is molecular mass,  $v$  is partial specific volume and  $N_o$  is Avogadro's number. Thereby,  $1-H = 0.62$  for  $h = 30\text{\AA}$  and  $M = 50 \text{ kDa}$ .) Then the enhancement in probability on addition of a fixed component becomes

$$\mathcal{E}_a = \{ [M(\text{total})_i / M(\text{total})_f] \times [M(\text{total})_f - M(\text{hetero})_i] / [M(\text{total})_i - M(\text{hetero})_i] \}^{1.46 \times C_{ave}-1}$$

(6)

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In the instance of a 50 kDa protein, half of which is heterogeneous, to which a 25 kDa Fv fragment is complexed,  $\mathcal{E}_a = \{ [50/75] \times [75-25] / [50-25] \}^{1.46 \times 4.5} - 1 = 5.6$ .

5 Thus if the overall crystallization probability of the protein was initially only 1 chance in 10, assuming all other crystallization probability components remained unchanged, the crystallization probability of the Fv fragment complex would be roughly 1 chance in 2, a substantial enhancement.

10

The accuracy of the quantification is only as good as the approximations, and several of the approximations used here call for further scrutiny. The approximation of molecular mass for surface area was used for the  
15 initial protein prior to heterogeneity removal. This is probably an underestimate since the completely heterogeneous portions of the protein would not be expected to fold as compactly as the homogeneous portions. In addition, the approximation that  $\partial \bar{n} \approx 0$   
20 tends to underestimate the deleterious influence of heterogeneity on crystallization. Both of these assumptions show an underestimation, but the equations still should predict the correct general trend. For some assumptions, however, the effect is more subtle.  
25 For example the equations were generated assuming one molecule per asymmetric unit. If one considered a tight complex of molecules, the same equations would hold as long as the complex did not have internal symmetry (complexes with internal symmetry show a different  
30 average contact number). Finally the category of heterogeneity is quite broad, and there are some situations, such as with segmental flexibility where these equations may be invalid. For example in the case of two rigid domains connected by a flexible linker, one  
35 would have to consider the possibility that one domain could be fixed relative to the other with a single appropriate contact.

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Increase of molecular variants. Another aspect of  
 variational crystallization, the use of multiple  
 variants of the same protein, also increases the  
 probability of crystal formation. In this case, the  
 5 overall probability of crystallization is exponentially  
 related to the number of variants. Assuming  
 independence of variants (a reasonable assumption with  
 different protein ligands; not as valid with minor  
 changes) with  $n$  variants and a probability of  
 10 crystallization for each variant of  $P_i$ , the overall  
 probability  $P_T$  is:

$$P_T = 1 - [(1-P_1) \times (1-P_2) \times \dots \times (1-P_n)] = 1 - \prod_{i=1}^n (1-P_i) \quad (7)$$

For example, if each variant of a relatively  
 heterogeneous protein had only a 25% chance of  
 crystallizing, the overall probability would be 1-  
 20  $(1-0.25)^n$ ; with 15 variants, the probability would  
 increase to almost 99%.

The enhancement in overall probability for successful  
 crystallization from a set of  $n$  variants can then be  
 25 calculated relative to the probability for a single  
 variant. If we assume that the probability for  
 crystallization of this individual variant,  $i$ , is  
 typified by the average for all variants,  $P_i \approx P_{ave}$ , the  
 enhancement factor is

$$\mathcal{E} = P_T / P_i - 1 \approx (1 / P_{ave}) - [(1-P_{ave})^n / P_{ave}] - 1 \quad (8)$$

If one tries many variants such that  $(1-P_{ave})^n \ll 1$ , then  
 the enhancement is inversely related to the average  
 35 probability of crystallizing a single variant:

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$$\mathcal{E} \approx (1/P_{ave}) - 1 \quad (9)$$

Thus, the more difficult a protein is to crystallize, the more it benefits from a strategy employing multiple variants.

5

### Experimental Procedures

Constructs of gp120. The various recombinant gp120 glycoproteins used for crystallization trials were produced in stable *Drosophila* Schneider 2 lines under the control of an inducible promoter as previously described(41) (Table 2). Genetic constructs containing various deletions and substitutions were made during the course of dissecting the gp120 domain structure. The procedures for making these constructs and the biological properties of the corresponding protein products are described elsewhere (see references in Table 2).

Protein production and purification. The N-terminal two domains of CD4 (D1D2), residues 1-183, were produced in Chinese hamster ovary (CHO) cells and purified as described previously(27). Human monoclonal antibodies 17b, A32, C11 and F105 (derived from HIV-infected individuals)(42,43) and mouse monoclonal antibodies L71 and 178.1(44,45) were purified by Protein-A affinity chromatography. Secreted gp120 from *Drosophila* cells was purified by affinity chromatography with the F105 antibody covalently coupled to Sepharose. Following extensive washing with phosphate-buffered saline containing 0.5 M NaCl, gp120 protein was eluted with 0.1 M glycine, pH 2.8, followed by immediate neutralization with Tris buffer.

Protease Digestion. Fab fragments were produced by papain digestion of monoclonal antibodies. Briefly, the antibody was reduced in 100 mM DTT, 100 mM NaCl, 50 mM

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Tris pH 8.0 for 1 hr at 37°C, and dialyzed (4°C), first in phosphate-buffered saline (PBS) to reduce the DTT concentration to ~1 mM, then in alkylating solution (PBS titrated to pH 7.5 with 2 mM iodoacetamide, 48 hr), and subsequently in PBS without iodoacetamide. The reduced and alkylated antibody was concentrated to at least 2 mg/ml and digested with papain using a commercial protocol (Pierce). An additional gel filtration chromatographic step on a Superdex S-200 column (Pharmacia, FPLC) was added to ensure oligomeric homogeneity.

The gp120 proteins were subjected to digestion with papain, elastase, and subtilisin (Boehringer Mannheim) to assay for proteolytic susceptibility. In these assays, the gp120 concentration was kept constant and the protease diluted serially (3.3x) from a ratio of 1:10 to 1:1000. The digestion mix was incubated for 1 hr at 37°C and quenched by addition of 1% SDS (1:10 ratio) with immediate heating in boiling water for 2 minutes. Digestion products were analyzed with SDS-polyacrylamide gel electrophoresis (PAGE) with and without DTT reduction.

Carboxypeptidase Y digestion was used to analyze the C-terminus of gp120. A 1:10 ratio of carboxylpeptidase Y (Boehringer Mannheim) to gp120 was incubated for 1 hr at 37°C, pH 7.0. Even though digestion could not be easily seen by SDS-PAGE, the C-terminus of gp120, HXBc2 strain, contains a number of positively charged amino acids, and the extent of the reaction could be monitored by native-PAGE.

Deglycosylation. *Drosophila*-produced gp120 proteins were deglycosylated enzymatically. Briefly, 0.5 mg/ml of gp120 was incubated with various deglycosylating enzymes (singly or in combination) in 0.5 M NaCl, 100 mM

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Na acetate, pH 5.7, for 10 hr at 37°C. Endoglycosidase D was used at a concentration of 0.1 U/ml, Endoglycosidase F at 0.25 U/ml, Endoglycosidase H at 0.25 U/ml, and Glycopeptidase F at 0.1 U/ml (all from Boehringer Mannheim). For crystallization variants involving the CD4-gp120 complex, the addition of D1D2 (which lacks carbohydrate) to the deglycosylation cocktail was found to enhance gp120 solubility. The deglycosylation reactions were monitored by following the reduction in molecular weight on SDS-polyacrylamide gel electrophoresis (SDS-PAGE). Deglycosylation was nearly complete within 30 min and plateaued after 3 hr. The extent of deglycosylation was judged by matrix-assisted laser desorption (MALDI) mass spectroscopy, carbohydrate analysis, affinity for concanavalin-A, and mobility and band width on SDS-PAGE. Protein aggregation was assayed by native-PAGE, dynamic light scattering, and gel filtration chromatography.

**Monoclonal antibody binding assay.** The various gp120 glycoproteins were assessed for recognition by a variety of monoclonal antibodies directed against both linear and discontinuous gp120 epitopes by either immunoprecipitation(46) or by ELISA(47). The ELISA was performed with both fully glycosylated and deglycosylated  $\Delta V1/2\Delta V3$  glycoproteins immobilized on ELISA plates using a capture antibody specific for the gp120 carboxyl-terminus, 6205 (International Enzymes) (47).

**Binary and ternary complex purification.** To ensure proper stoichiometry and oligomeric homogeneity, all complexes were purified by gel filtration chromatography on a Superdex S-200 column (Pharmacia, FPLC). This column exhibited good resolution with routine separation of samples that differed by only 30% in molecular weight. Individual components were first purified



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separately to ascertain their monomeric status. Components were then combined to form complexes, which were repurified on the same column. A buffer of 0.35 M NaCl, 5 mM Tris/Cl pH 7.0, 0.02% NaN<sub>3</sub> was used throughout. Peak fractions were concentrated over centricon-30 (Amicon) to a final protein concentration of ~10 mg/ml and either aliquoted and stored at -80°C or used directly for crystallization.

10 Crystallization. The vapor-diffusion hanging-droplet technique was used for all crystallizations. Small volumes, 0.5 µl protein solution + 0.5 µl reservoir solution, were used for most crystallizations, screenings and final optimizations.

15 Screening. The Crystal Screen I (Hampton Research) was used, augmented by approximately 20 conditions which tested high protein concentrations (vapor diffusion concentration of the protein at various pHs) as well as mixtures of organic additives (2-5% MPD, PEG 400, or PEG 20 4000) combined with high ionic strength (2-4 M NaCl, (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> or Na/KPO<sub>4</sub>) at pH 5.5-9.5. For each gp120 crystallization variant, a subset of 12 different conditions was analyzed in depth to establish the approximate precipitation point of the protein for a 25 variety of different precipitants. The factorial solutions were then individually adjusted to target the observed precipitation point and a full screen of ~70 conditions was set up at 20°C. After at least one week of constant daily observation, screening solutions were 30 recalibrated to account for the observed 20°C precipitation point and another full screen at 4°C was set up. If no crystals were observed, the Crystal Screen II (Hampton Research) was set up at 20°C.

35 Optimization. In addition to the standard single variable optimization of crystallization conditions, a

factorial-like procedure was used to determine if small amounts of different additives increased crystal quality. Type E crystals were grown from the following conditions: Protein ( $\Delta 82\Delta V1/2 * \Delta V3\Delta C5$  gp120, two-domain CD4 (D1D2), Fab 17b purified as a ternary complex on the Superdex S-200); Droplet (0.5  $\mu$ l protein solution consisting of ~10 mg/ml protein in gel filtration buffer + 0.4  $\mu$ l droplet mix containing 0.1 M NaCitrate, 0.02 M NaHepes, 10% isopropanol, 10.5% PEG 5000 monomethylether (Fluka), 0.0075% SeaPrep Agarose (FMC BioProducts), pH 6.4; Reservoir: (0.35 M NaCl, 0.1 M NaCitrate, 0.02 M Hepes, 10% isopropanol, 10.5% PEG 5000 monomethylether, pH 6.4). The droplet mix was kept at 37°C to ensure the agarose solubility, and the crystallization setup at room temperature. Clumps of crystals appeared within two weeks of incubation at 20°C and grew for several months to maximal size.

X-ray diffraction characterization. All data were collected at beamline X4A of the National Synchrotron Light Source, Brookhaven National Laboratory. The type E crystals were crosslinked with the vapor diffusion technique of Lusty(48) by placing a crystallization bridge (Hampton Research) with a 25  $\mu$ l sitting droplet of 1% glutaraldehyde (Sigma) in the reservoir of a standard hanging droplet vapor diffusion crystallization setup for 1 hr at room temperature. The crosslinked crystal was washed with stabilizer (reservoir solution with only 50 mM NaCl) containing 10% ethylene glycol. After approximately 24 hr, the external liquid surrounding the crystal was replaced with paratone-N (Exxon), the crystal mounted in an ethylene loop (Hampton Research) (49), and flash-cooled in the nitrogen stream of a cryostat (details are provided in (50)). Oscillation data were processed with DENZO(51) and scaled with SCALEPACK(51).

## Results and Discussion

To address the many problems associated with the crystallization of HIV-1 gp120, we exploited the mutability of the macromolecular surface using tactics that involved protein modification and conformational restriction (Table 3). Several of these tactics contain novel features and are detailed here.

Variant constructs of the gp120 protein. Variants of gp120 were developed through an iterative cycle which strove to eliminate heterogeneity. The cycle involved recombinant production of gp120 variants, deglycosylation, and then assessment of heterogeneity and flexibility by examinations of glycosylation status, monoclonal antibody binding, and protease sensitivity, leading to the design of new constructs. For example, protease digestion monitored by PAGE indicated susceptibility at the C-terminus, and a form with 15-20 residues removed by carboxypeptidase Y retained CD4 binding activity. A homogeneous product was difficult to make by this method, and primer-based PCR mutagenesis and recombinant expression were used to generate a homogeneous gp120 derivative with a 19-residue C-terminal deletion. At the N-terminus, sequencing of the initial constructs showed the expected signal cleavage at +31, with four additional amino acids, Gly-Ala-Arg-Ser, added from the signal peptide (a consequence of different processing of the cloning vector signal peptide with gp120). Protease digestion gave a product at +40, indicating flexibility in the N-terminus. Progressive genetic truncation and biochemical analysis identified +83 as a variant that was recognized by conformation-dependent gp120 ligands, whereas +94 exhibited some conformational disruption(46). Thus much of the apparently flexible region at the N-terminus of gp120 could be removed

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without disrupting the global conformation of the protein.

To further reduce flexibility, variable loops, V1, V2, and V3, were deleted and replaced with shorter segments, as reported earlier (52,53). Little effect was found on CD4 binding activity(47,53). Three constructs were made which contained deletions of the V1, V2, and V3 loops (Table 2). In the  $\Delta V1/2\Delta V3$  construct, the entire base and stem of the variable loops V1, V2 and V3 were excised. In the  $\Delta V1/2*\Delta V3$  protein, the conserved stem of the V1/V2 stem-loop structure was retained, restoring the CD4-induced antibody epitopes in the presence of soluble CD4. In the  $\Delta V1/2*\Delta V3^*$  protein, the base of the V3 loop was retained as well, fully restoring CD4-induced antibody epitopes, even in the absence of soluble CD4.

Deglycosylated forms of gp120. The asparagine-linked carbohydrate on the gp120 glycoprotein produced in *Drosophila* cells was analyzed. Dionex chromatography showed that the carbohydrate on this protein consisted of (N-acetyl-glucosamine)<sub>2</sub> (fucose)<sub>F</sub> (mannose)<sub>M</sub>, with F = 0 or 1 and M = 3 to 9 (JSC, unpublished data). Deglycosylation with enzymes such as Glycopeptidase F (or Endoglycosidase F at pH 5.0), which cleave the glycosidic linkage and convert the N-linked asparagine into an aspartic acid, resulted in gp120 aggregation, although it remained soluble. Cleavage of the 1-4  $\beta$ -bonds in the chitobiose core with Endoglycosidases D or H, leaving only a single N-acetylglucosamine residue and, potentially, a 1-6 fucose attached to any of the glycosylated asparagine residues, appeared to leave the protein intact as judged by a panel of conformationally sensitive monoclonal antibodies(47). Digestion of full-length constructs with Endoglycosidase H, which has specificity for oligosaccharides with 5-9 mannose

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residues, removed roughly 60% of the carbohydrate, and addition of Endoglycosidase D, which cleaves oligosaccharides with 3 or 4 mannose residues, removed up to 90% of the carbohydrate. For the variable  
5 loop-deleted constructs, all mannose residues were removed with the Endoglycosidase D/H combination as judged by carbohydrate analysis and by the inability of concanavalin A to bind to the deglycosylated protein. Mass spectroscopy of the deglycosylated  $\Delta 82\Delta V1/2*\Delta V3\Delta C5$   
10 gp120 showed a molecular mass of  $39,000 \pm 50$  Da, consistent with a mass of 35.4 kDa for the protein (based on the DNA sequence) and 3.6 kDa for the remaining carbohydrate. Carbohydrate analysis showed only fucose and N-acetyl-glucosamine sugars to be  
15 present, in a ratio of  $1:3.05 \pm 0.02$ , respectively. These results suggest that, of the 18 potential asparagine glycosylation sites in the  $\Delta 82\Delta V1/2*\Delta V3\Delta C5$  gp120, five are unused, nine are modified with N-acetyl-glucosamine and four with N-acetyl-glucosamine  
20 (1-6) fucose.

Complexes with gp120 ligands. Protein ligands, CD4 and the Fab fragments of monoclonal antibodies, were used in an attempt to reduce mobility in the overall surface of  
25 the protein and, hence, in the potential crystal lattice. This was complicated by the internal mobility of these ligands: CD4 has a flexible juncture between the second and third extracellular domains(54), and Fabs have a conformationally mobile "elbow bend" between  
30 their variable and constant domains(55). For CD4, we used a construct containing the N-terminal two domains (1-182), for which we had previous success in structure determination(27). Fabs of the monoclonal antibodies, were screened individually, even though combinations of  
35 Fabs were possible.

Initial trials with the Fab 178.1, which recognizes a

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linear epitope in V3 of both free- and CD4-bound gp120(44), gave only crystalline precipitates at best. We also tested the Fab of the anti-CD4 antibody L71, which recognizes the CDR3-like loop in domain D1(45),  
5 but had difficulties preparing ternary complexes, probably due to a destabilization of the CD4 - gp120 interaction. Subsequently, we focused on gp120-directed antibodies with discontinuous epitopes, which were more likely to recognize conformationally rigid portions of  
10 gp120. Complexes of gp120 proteins with Fabs of C11, which recognizes an epitope spanning C1 and C5(42), and F105, whose epitope lies within C2, C3, C4, and C5 (overlapping the CD4 binding site)(43) gave only poor crystals (Table 4). We had greater success with 17b,  
15 which not only recognizes a discontinuous epitope but discriminates between different conformational states of gp120(36). The Fab of 17b did not bind the initial gp120 constructs, requiring the restoration of the stem of the V1/V2 loop (constructs  $\Delta V1/2*\Delta V3$  or  $\Delta V1/2*\Delta V3^*$ ).

20

Crystallization. We screened 18 different combinations of gp120 variants and ligands (Table 4), using a limited factorial-based crystallization screen. Factorial screening was originally devised as a method for  
25 deducing the essential crystallization factors from combinations of different conditions(1). The empirical observation, however, that most crystallizable macromolecules are able to crystallize from a limited set of common conditions, has validated an entirely  
30 different process: crystallization screening with a small but diverse collection of fixed conditions(2). A high probability of success has been reported with as few as 6 different conditions at 4 different concentrations(56), and commercial kits are available  
35 with 50-100 conditions (Hampton Research).

In conjunction with the limited crystallization screen,

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small volume droplets were used, typically 0.5  $\mu$ l of protein per crystallization trial. With small volumes, 1-2 mg of protein was sufficient to evaluate each gp120 crystallization variant. Smaller volumes were also more efficient at nucleation than larger droplets, perhaps due to higher surface tension effects which may result in a greater range of precipitant concentrations for each droplet to sample. Indeed, droplets that were "spread-out" also showed enhanced nucleation. This explanation may also account for the well-known observation that crystals frequently nucleate from the edges of crystallization droplets.

The initial crystallization screens produced six different types of crystals (Fig. 1, Table 5). For crystal types A-D, extensive optimization was unable to produce single crystals large enough to be characterized. For crystal types E and F, single crystals of needle morphology could be grown. The growth of single crystals of type E, however, required the addition of agarose, which was identified during optimization by the additive screening process. Trials with a variety of agaroses found the SeaPrep, with a gelling point near room temperature, gave the best results. Despite considerable effort, further crystallization optimization failed to produce large single crystals, and the best typical crystals were rods with a cross-section of only 30 x 40  $\mu$ m. A closely related crystallization variant, which retained 10 additional amino acids in the stem of the V3 loop, failed to crystallize (Table 4).

Characteristics of gp120 crystals. Single crystals of type E and F were analyzed for diffraction in capillary mounts. Only type E crystals showed diffraction. The needle axis of type E crystals proved to coincide with the a axis, and the rhombohedral cross-section

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perpendicular to the needle axis proved to be bounded by faces of the form (0 1 1). These could be distinguished from type F crystals, where the cross-section was hexagonal. Gel electrophoresis of type E crystals demonstrated that they contained all the elements of the ternary complex: gp120, D1D2, and Fab 17b (Fig. 2).

We were unable to flash-cool the type E crystals with standard cryoprotectants. Satisfactory results were found with a procedure that (i) fortified the crystals with vapor-diffusion glutaraldehyde crosslinking(48), (ii) permeated the crystals with 10% ethylene glycol and (iii) used an immiscible oil, paratone-N, to replace the external solution around the crystals prior to flash-cooling(50). Cryopreserved crystals diffracted to Bragg spacings of better than 2 Å, although the diffraction was anisotropic, with higher mosaicity along the 88 Å *b*-axis.

Type E crystals were orthorhombic, space group P222<sub>1</sub>, with unit cell parameters,  $a=71.25\text{\AA}$ ,  $b=88.11\text{\AA}$  and  $c=196.44\text{\AA}$  ( $\alpha=\beta=\gamma=90^\circ$ ). Solvent content analysis yielded a solvent content of 58% for one ternary complex in the crystallization asymmetric unit (assuming a partial specific volumes of 0.73 for protein and 0.65 for carbohydrate and the observed total molecular mass of 108.3 kDa for the complex of which 3.6 kDa is carbohydrate). Diffraction data have been collected to a limit of 2.2 Å spacings (Table 6).

**Conclusions.** Our success with gp120 demonstrates the power of variational crystallization. We have derived equations that quantify the effect of this strategy on the overall probability of crystallization and have calculated the corresponding probability enhancements for several of the biochemical and molecular biological manipulations employed in this study. As can be seen



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(Table 3), the probability of crystallization can be strongly influenced by reducing molecular surface heterogeneity. The influence of using multiple variants is more difficult to quantify since it depends on the individual probability of crystallization for each variant. Nonetheless, our theoretical analysis shows that the effect of multiple variants is greatest for proteins least likely to crystallize.

10

While the variational approach with gp120 did involve extensive effort, this was primarily a consequence of the difficulty in producing the gp120 glycoprotein, which involved expression levels of only a few mg of gp120 per liter of eukaryotic cell culture. While future advances in molecular biology will no doubt make such projects less arduous, if proteins are expressed bacterially, present day recombinant techniques coupled to affinity or "tag" purifications make the generation of variants straightforward. A recent example, involving the generation of 11 different variants in the crystallization of an ionotropic glutamate receptor(57), required only a 6 month effort (E. Gouaux, personal communication).

25

The resistance of gp120 to crystallization may be related in part to its functional role in eluding the immune system; the mechanisms evolved to prevent the formation of specific immune system : gp120 contacts, might also thwart formation of the homogeneous gp120 : gp120 contacts needed for crystallization. Perhaps relevant to this, the protein modifications that most greatly reduced heterogeneity (and thus enhanced the crystallization probability), removal of carbohydrate and substitution of the variable loops (Table 3), have been shown in vivo to enhance the generation of neutralizing antibodies(58,59).

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It is difficult to evaluate the predictions of the crystallization algorithms derived here in a statistically significant manner. The failure of proteins to crystallize is rarely reported in the literature, and our own results comprise too small a sample to be statistically meaningful. Nonetheless, we note that for gp120 the algorithms predict that crystals are most probable with deglycosylation, variable loop removal, and addition of an ordered protein ligand. Consistent with prediction, for the 6 crystallization variants that did have all of these modifications, three (or 50%) produced crystals, whereas for the 12 variants that did not have these modifications, no crystals (0%) were grown. In addition, theory predicts that well-ordered crystals are most probable when the overall probability of crystallization is highest; Table 4 shows that the crystallization variant that produced the only well-ordered crystals appeared to have the greatest probability of crystallization, producing three different crystals forms whereas the best of the other variants only produced one form each.

The crystallization literature is replete with examples of protein manipulation, from proteolytic digestion, to variation in solvating detergent, to screening of DNA oligonucleotides(38). What distinguishes our efforts is the derivation of a theoretical foundation, which allows the probabilistic assessment of the most effective crystallization approach. Because of the conformational complexity of gp120, we focused on surface modification -- to eliminate heterogeneity and to present new crystallization variants -- coupled to a limited screen of crystallization conditions. The types of crystallization problems embodied in gp120 (Table 3) are not so different from many of the typical problems facing present day crystallographers; both from a theoretical or from a practical perspective, the

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strategy of probability analysis coupled to variational crystallization may be broadly applicable.

5 Subsequent to the submission of this manuscript, the structure determination of type E crystals was reported(63).

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† Estimate of the effect on the crystallization probability of a strategy which optimizes the particular factor. The number of (+) symbols denotes the size of the effect: (+) refers to almost no change in probability after optimization, whereas (+++++) refers to a large change in probability. The scale used here is a qualitative estimate; for more quantitative results, see Table 3. For chemical heterogeneity, optimization refers to the effect on crystallization of making the protein more chemically homogeneous. For conformational heterogeneity, optimization refers to the effect of removing or circumventing the particular source of heterogeneity.

Table 2. The gp120 constructs used for crystallization.

construct name	gp120 strain <sup>†</sup>	amino acid for construct <sup>§</sup>	reference
$\Delta 61$ -III <sub>B</sub>	III <sub>B</sub>	62-511	(59)
$\Delta 30$ -FL	JRFL	31-511	(60)
$\Delta V1/2\Delta V3$	BH10/HXBc2	31-120 GAG 204-297 GAG 330-511	(53)
$\Delta V1/2\Delta V3\Delta C5$	BH10/HXBc2	31-120 GAG 204-297 GAG 330-492	(61)
$\Delta 82\Delta V1/2*\Delta V3\Delta C5$	HXBc2	83-127 GAG 195-297 GAG 330-492	(61)
$\Delta 82\Delta V1/2*\Delta V3*\Delta C5$	HXBc2	83-127 GAG 195-302 GAG 325-492	(61)

<sup>†</sup> The  $\Delta V1/2\Delta V3$  and  $\Delta V1/2\Delta V3\Delta C5$  constructs were chimeras of strains BH10 and HXBc2.

<sup>§</sup> Sequence numbers refer to the translated gp160, with the mature gp120 beginning at +31. N-terminal sequencing showed that all constructs contained 4 additional amino acids, Gly-Ala-Arg-Ser, an artifact of the signal peptide cleavage. GAG here refers to the tripeptide, Gly-Ala-Gly, which was substituted for the removed amino acids.

**Table 3.** Crystallization problems, variational crystallization solutions, and enhancement of crystallization probability.

Problem	Solution	Probability Enhancement <sup>†</sup>
N-linked carbohydrate	Protein production in an inducible <i>Drosophila</i> cell line coupled with deglycosylation with Endoglycosidases D and H	1200%
Surface loop flexibility	Replacement of V1/V2 and V3 loops with tripeptide linkers of Gly-Ala-Gly.	370%
N- and C- terminal heterogeneity	Mutational deletion and proteolytic cleavage analysis coupled to the production of gp120 with truncated N- and C-termini	50% <sup>§</sup>
Conformational heterogeneity	Conformation restriction with protein ligands such as CD4 and Fabs from conformationally sensitive monoclonal antibodies	$(1/P_{ave}) - 1$ <sup>¶</sup>

<sup>†</sup> The probability enhancement,  $\epsilon$ , was calculated from the equation:

$$([MW(\text{total})_i / MW(\text{total})_f]^{1.46} \times C_{ave} - 1)$$
 with  $C_{ave} = 4.5$ , the average observed contact number. For the drosophila produced HXBc2, the molecular weight for the glycosylated gp120 is approximately 90 kDa; the deglycosylated gp120, 60 kDa; and the deglycosylated  $\Delta V1/2\Delta V3$  gp120, 47 kDa.

<sup>§</sup> The N- terminus is resistant to proteolysis from +39 to +82, and thus probably adopts an ordered conformation. This number was calculated assuming only the C-terminal 19 and the N-terminal 8 amino acids were disordered.

<sup>¶</sup> Dependent on the average probability ( $P_{ave}$ ) of crystallizing a single variant of gp120. If  $P_{ave} = 10\%$ , the use of many variants would lead to a probability enhancement of 900%.

Table 4. Summary of HIV-1 gp120 crystallization attempts

HIV-1 gp120 construct	glycosylation status §	cofactors †	comments #
$\Delta 61$ -III B (III B strain)	glycosylated	—	bad precipitates
	~60% deglycosylated	—	bad precipitates
	~90% deglycosylated but some Asn to Asp	—	precipitates look better but still primarily bad
	~60% deglycosylated	D1D2 sCD4	ok precipitates
	~60% deglycosylated	Fab 178.1	ok precipitates
	~60% deglycosylated	D1D2 sCD4 and Fab 178.1	ok precipitates
	~90% deglycosylated	—	ok precipitates
$\Delta 30$ -FL (JRFL strain)	~90% deglycosylated	—	ok precipitates
		D1D2 sCD4	ok to good precipitates
		Fab 178.1	good precipitates
		D1D2 sCD4 and Fab 178.1	good precipitates -- no crystals
$\Delta V1/2\Delta V3$ (BH10/HXBc2 strain)	fully deglycosylated	—	good precipitates -- no crystals
		D1D2 sCD4	very small, nice looking crystals in PEG 400 (Crystal Type A)
		D1D2 sCD4 and Fab C11	badly formed crystals from $(\text{NH}_4)_2\text{SO}_4$ (Crystal Type B)
$\Delta V1/2\Delta V3\Delta C5$ (BH10/HXBc2 strain)	fully deglycosylated	D1D2 sCD4	spheroidal crystals in PEG 4000 (Crystal Type C)
		Fab F105	good precipitates -- no crystals
$\Delta 82\Delta V1/2*\Delta V3\Delta C5$ (HXBc2 strain)	fully deglycosylated	D1D2 sCD4 and Fab 17b	three different types of crystals (Types D-F). Orthorhombic diffract to at least 2.2 Å
$\Delta 82\Delta V1/2*\Delta V3*\Delta C5$ (HXBc2 strain)	fully deglycosylated	D1D2 sCD4 and Fab 17b	good precipitates -- no crystals

†D1D2 sCD4 refers to two-domain soluble CD4. Antibody epitopes are described in the text..

§The percent deglycosylation reported here refers to the percent of N-linked sites cleaved by endoglycosidase D or H. Thus the "fully deglycosylated" protein still contains N-acetyl glucosamine and fucose additions.

#The correlation between overall physical characteristics of a precipitate in a crystallization trial and the actual crystallization probability are imprecise. As a consequence, the comments made here describing precipitates are extremely qualitative. "Bad precipitates" indicate that most of the precipitates were yellow to light-yellow in color, indicative of denatured protein. "Good precipitates" indicates that in some conditions, the precipitates appeared to be microcrystalline, but individual crystals could not be discerned. "Ok precipitates" span the continuum between these two extremes.

Table 5. Crystallization conditions for initial gp120 crystals.

Crystal Type	Protein †	Concentration §	Reservoir Solution ¶
A	$\Delta V1/2\Delta V3$ D1D2 sCD4	14.0	30% PEG 400, 0.2 M $MgCl_2$ , 0.1 M Na Hepes pH 7.5 (reagent 23)
B	$\Delta V1/2\Delta V3$ D1D2 sCD4 Fab C11	9.2	2 M $(NH_4)_2SO_4$ , 2% PEG 400, 50 mM $MgCl_2$ 50 mM Tris pH 8.5
C	$\Delta V1/2\Delta V3\Delta C5$ D1D2 sCD4	11.0	6.7% PEG 4000, 3.3% isopropanol, 33 mM Na Hepes pH 7.5 (3-fold dilution of reagent 41)
D	$\Delta 82\Delta V1/2*\Delta V3\Delta C5$ D1D2 sCD4 Fab 17b	7.6	15% PEG 4000, 0.1 M $NH_4$ Acetate 50 mM Na Citrate pH 5.6 (2-fold dilution of reagent 9)
E	$\Delta 82\Delta V1/2*\Delta V3\Delta C5$ D1D2 sCD4 Fab 17b	7.6	10% PEG 4000, 10% isopropanol 50 mM Na Citrate pH 5.6 (2-fold dilution of reagent 40)
F	$\Delta 82\Delta V1/2*\Delta V3\Delta C5$ D1D2 sCD4 Fab 17b	6.6	6.7% PEG 8000, 15% isopropanol, 67mM $MgCl_2$ 33 mM Na Cacodylate pH 6.5 (3-fold dilution of reagent 18)

† All binary and ternary complexes were purified by gel filtration. D1D2 sCD4 refers to the two domain soluble CD4.

§ The protein concentration is given as the absorbance (280 nm) of the complex per ml of solution.

¶ Most of the reservoirs are conditions from Crystal Screen 1 (Hampton Research); the reagent numbers given here refer to the crystallization reagent from this commercial kit. Hanging droplets were 0.5  $\mu$ l protein (in 0.35 M NaCl, 5 mM Tris pH 7.0, 0.02%  $NaN_3$ ) + 0.5  $\mu$ l reservoir, except for crystal type B, which used 0.5  $\mu$ l of 3-fold diluted reservoir. Crystallization reservoirs were 500  $\mu$ l; an additional 35  $\mu$ l of 5 M NaCl was added after the droplet was mixed to compensate for the NaCl in the protein solution. All dilutions used  $H_2O$ , except for crystal type F, where 22.5% isopropanol was used. Crystallizations were setup at room temperature and incubated at 20°C.

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**Table 6.** Data collection statistics for Type E crystals of the two-domain CD4 (D1D2)/ Fab 17b /  $\Delta 82\Delta V1/2*\Delta V3\Delta C5$  gp120 complex.

	drange (Å)	# reflections (unique)	R sym (%)	Completeness (%)
all data	20-2.2	56,195	14.5	87.4
last shell	2.48-2.2	13,928	35.5	73.1

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TABLE 7

	<u>PROTEIN*</u>	<u>CONC</u>	<u>RESERVOIR SOLUTION**</u>	<u>μlP</u>	<u>μlR</u>	<u>FIGURE</u>
5	A	11.0	Factorial 1 #40 500μl factorial/ 880μl Total vol. (1.76 dilution)	0.5	0.35	5 A,B
10			Factorial 1 #28 500μl factorial/1375μl Total vol. (2.75 dilution)	0.5	0.35	6
15			* Factorial 1 #18 500μl/1375 total volume (2.75 dilution)	0.5	0.35	7
20			Factorial 1 #14 +50μl 100% PEG 400 500μl/550μl total volume (50μl of PEG only)	0.5	0.35	8
25			Factorial 1 #43 + 200μl Saturated AM <sub>2</sub> SO <sub>4</sub> 500μl only/700 μl total vol.	0.5	0.35	9
30			PS Factorial #46 200μ factorial/ 600μl total volume	0.5	0.35	10
35			PS Factorial #31 200μl factorial/ 550μl total volume (2.75 dilution)	0.5	0.5	11
40	B	5.2	Factorial 1 #18 +50μl pH 4.5 Na Acetate 0.5M / 250μl factorial/ 688 total volume	0.5	0.35	12
45			PS Factorial #26 200μl factorial/ 800μl total volume (4.0 dilution)	0.5	0.5	13
50			PS Factorial #28 200μl factorial/ 400μl total volume (2.0 dilution)	0.5	0.5	14

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	G	1.36	PS Factorial #35 200µl factorial/ 700µl total volume	0.5	0.5	15
5	M	1.4	PS Factorial #9 200µl factorial/ 200µl total volume	0.5	0.5	16
10			Factorial 1 #32 500µl factorial/ 900µl total volume	0.5	0.35	17
15	N	6.2	Factorial 1 #17 500µl factorial/ 1300µl total volume	0.5	0.35	18
20			Factorial 1 #18 500µl factorial/ 1300µl total volume	0.5	0.35	19
25			Factorial 1 #38 500µl factorial/ 1000µl total volume	0.5	0.35	20
30		*	Factorial 1 #40 500µl factorial/ 1200µl total volume	0.5	0.35	21
35			Factorial 1 #46 500µl factorial/ 900µl total volume	0.5	0.35	22
40			PS Factorial #12 200µl factorial/ 300µl total volume	.05	0.5	23
			PS Factorial #29 200µl factorial/ 500µl total volume	.05	0.5	24
45			Factorial 1 #40 + Factorial 1 # 16 150µl #16 250µl #40/600µl total vol.	0.5	0.35	25
50		*	Crystals gave good diffraction			
		**NOTE:	To all reservoirs 5M NaCl was added to bring the final concentration to 350mM. after droplet set up.			
			The final volume was made up by water, if there is a volume discrepancy.			



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## Second Series of Experiments

The human immunodeficiency viruses (HIV-1 and HIV-2) and simian immunodeficiency viruses (SIVs) are the etiologic agents of acquired immunodeficiency syndrome (AIDS) in their respective human and simian host (1). Typically, infection with primate immunodeficiency viruses is characterized by an initial phase of high-level viremia, followed by a long period of persistent virus replication at a lower level (2). Viral persistence occurs despite specific antiviral immune responses, which include the generation of neutralizing antibodies.

The primate immunodeficiency viruses, like all retroviruses, are surrounded by an envelope consisting of a host cell-derived lipid bilayer and virus-encoded envelope glycoproteins (3). For the virus to enter target cells, the viral membrane must be fused with the plasma membrane of the cell, a process mediated by the envelope glycoproteins. The exposed location of these proteins on the virus allows them to carry out their function but also renders them uniquely accessible to neutralizing antibodies. Thus, dual selective forces, virus replication and immune pressure, have shaped the evolution of the envelope glycoproteins and continue to do so within each infected host. Below summarized the current understanding of the functional features of these proteins.

### Synthesis and assembly of the envelope glycoproteins.

In the infected cell, the envelope glycoproteins are synthesized as approximately 845-870 amino acid precursor in the rough endoplasmic reticulum. (N)-linked, high-mannose sugar chains are added to form the gp160 glycoprotein, which assembles into oligomers (4-6). The preponderance of evidence suggests that these oligomeric complexes are trimers (4,5). The gp160

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trimers are transported to the Golgi apparatus, where cleavage by a cellular protease generates mature envelope glycoproteins: gp120, the exterior envelope glycoprotein, and gp41, the transmembrane glycoprotein (3). The gp41 glycoprotein possesses an ectodomain that is largely responsible for trimerization (7), a membrane-spanning anchor, and a long cytoplasmic tail. Most of the surface-exposed elements of the mature, oligomeric envelope glycoprotein complex are contained on the gp120 glycoprotein. Selected, presumably well-exposed, carbohydrates on the gp120 glycoprotein are modified in the Golgi apparatus by the addition of complex sugar (6). The gp120 and gp41 glycoproteins are maintained in the assembled trimer by non-covalent, somewhat labile interactions between the gp41 ectodomain and discontinuous structures composed of N- and C-terminal gp120 sequences (8). Upon reaching the infected cell surface, a fraction of these envelope glycoproteins complexes are incorporated into budding virus particles. A large number of the complexes disassemble, releasing gp120 and exposing the previously buried gp41 ectodomain. These events contribute to the formation of defective virions, which predominate in any retroviral preparation (9).

Binding of the envelope glycoproteins to the CD4 receptor.

Many cell surface proteins, including adhesion molecules, are incorporated into HIV-1 virions along with the envelope glycoprotein complexes (10). These host cell-derived molecules can assist the attachment of viruses to potential target cells. Virus attachment also involves the interaction of the gp120 envelope glycoproteins with specific receptors, the CD4 glycoprotein (11) and members of the chemokine receptor family (12, 13) (Fig. 26). The CD4 glycoprotein is expressed on the surface of T lymphocytes, monocytes,

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dendritic cells, and brain microglia, the main target cells for primate immunodeficiency virus in vivo. The requirement for CD4 binding exhibited by most primate immunodeficiency viruses for efficient entry is  
5 consistent with this observed in vivo tropism. A major function of CD4 binding is to induce conformational changes in the gp120 glycoprotein that contribute to the formation and/or exposure of the binding site for the chemokine receptor (13, 14). Some HIV-1 and HIV-2  
10 isolates cultured in the laboratory, as well as several primary SIV isolates, no longer depend upon CD4 for efficient entry, and bind to chemokine receptors but not CD4 for interaction (15). These examples and the observation that feline immunodeficiency viruses use  
15 chemokine receptors but not CD4 for entry (16) raise the distinct possibility that the chemokine receptors represent the primordial, obligate receptors for this retroviral lineage. The use of CD4 as a receptor may have evolved subsequently, allowing the high-affinity  
20 chemokine receptor-binding site of primate immunodeficiency viruses to be sequestered from host immune surveillance.

Multiple approaches have yielded insights into the  
25 structural basis for CD4-binding by the primate immunodeficiency virus gp120 glycoproteins. Early comparisons of gp120 sequences revealed the existence of five variable (V1-V5) regions interspersed with five conserved regions (17). Intramolecular disulfide bonds  
30 in the gp120 glycoprotein result in the incorporation of the first four variable regions into large, loop-like structures (6). Antibody binding studies and deletion mutagenesis have indicated that the major variable loops are well-exposed on the surface of the gp120  
35 glycoprotein (18, 19). The more conserved regions fold into a gp120 core which has been recently crystallized in a complex with fragments of CD4 and a neutralizing

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antibody (20). The gp120 core is composed of two domains, an inner domain and an outer domain, and a  $\beta$  sheet (the "bridging sheet") that does not properly belong to either domain (Fig. 27a). These names reflect the likely orientation of gp120 in the assembled envelope glycoprotein trimer: the inner domain faces the trimer axis and, presumably, gp41, while the outer domain is mostly exposed on the surface of the trimer. Elements of both domains contribute to CD4 binding. CD4 binds in a recessed pocket on gp120, making extensive contact over approximately 800 Å<sup>2</sup> of the gp120 surface. Two cavities are evident in the gp120-CD4 interface. A shallow cavity is filled with water molecules, while a deep cavity extends 10-15 Å into the interior of gp120. The opening of this deep cavity is occupied by phenylalanine 43 of CD4, which has been shown by mutagenic analysis to be critical for gp120 binding (21). Most of the gp120 residues previously identified as important for CD4 binding (22,23) surround the opening of the deep cavity and contribute to interactions with phenylalanine 43 of CD4. In addition, aspartic acid 368 of gp120 forms a salt bridge with arginine 59 of CD4, also shown by mutagenesis to be important for gp120 binding (21). Additionally, mainchain atoms on gp120 and CD4 form hydrogen bonds bridging the two proteins. The formation of the deep cavity in gp120 likely contributes to the transmission of CD4-induced conformational changes to gp120 elements involved in the interaction with chemokine receptors and/or gp41. The deep cavity may be a useful target for intervention by small molecular weight compounds.

#### Chemokine receptor binding

Most primary, clinical isolate of primate immunodeficiency viruses use the chemokine receptors CCR5 for entry (12). For most HIV-1 isolated that are transmitted and that predominate during the early years

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of infection, CCR5 is an obligate coreceptor, and rare individuals that are genetically deficient in CCR5 expression are relatively resistant to HIV-1 infection (24). HIV-1 isolates arising later in the course of infection often use other chemokine receptors, frequently CXCR4, in addition to CCR5 (12,24). Studies of chimeric envelope glycoproteins demonstrated that the third variable (V3) loop of gp120 is a major determinant of chemokine receptor choice (12,25). V3-deleted versions of gp120 do not bind CCR5, even though CD4 binding occurs at wild-type levels (14). Antibodies against the V3 loop interfere with gp120-CCR5 binding (14). These results support an involvement of the V3 loop in chemokine receptor binding. Other, conserved gp120 structures also appear to play an important role in chemokine receptor binding. The use of CCR5 by a diverse group of immunodeficiency viruses with divergent V3 sequences, first suggest the involvement of more conserved gp120 elements (26). Antibodies that recognize conserved, discontinuous gp120 epitopes that are more exposed after CD4 binding are potent inhibitors of gp120-CCR5 interaction (14). These CD4-induced (CD4i) epitopes are discussed further below. Recent mutagenic and structural analysis have revealed the existence of a highly conserved gp120 structure that is important for CCR5 binding (20,27) (Fig. 27, a and b). This structure is adjacent to the V3 loop and the CD4i epitopes, and is oriented to face the target cell upon gp120-CD4 binding.

#### gp41-mediated membrane fusion.

It is likely that the interaction of the gp120-CD4 complex with the appropriate chemokine receptor promotes additional conformational changes in the envelope glycoprotein complex. By analogy with the influenza hemagglutinin, it has been suggested that the HIV-1 gp41 ectodomain undergoes major conformational changes during

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virus entry (28). The proposed result of these changes is the insertion of the hydrophobic gp41 amino terminus (the "fusion peptide") into the membrane of the target cell. Mutagenic analysis (23,29) and the recently  
5 determined crystal structures of HIV-1 gp41 ectodomain fragments (5) are consistent with this model. The gp41 ectodomain structures reveal an extended, trimeric coiled coil that could potentially bridge the viral and target cell membranes (5). Interactions of other gp41  
10 helical segments near the membrane-spanning region with the interhelical grooves of the internal coiled coil are important for fusion-related conformational changes in gp41. This interaction can be inhibited by helical peptides that mimic either of the involved gp41 helices  
15 (30) and is a potential target for future intervention with small molecular weight compounds.

The HIV-1 envelope glycoproteins as antigens.

The exposure of the primate immunodeficiency virus  
20 envelope glycoproteins on the surface of virions or infected cells makes them prime targets for antibodies that potentially block key functions of these proteins. However, the success of these viruses in achieving persistent infections implies that the viral envelope  
25 glycoproteins have evolved to be less-than-ideal immunogens and antigens. Structures on the viral envelope glycoproteins that are conserved among diverse viral strains are, in general, poorly exposed to the humoral immune system. The conserved gp120 surfaces  
30 involved in binding to its three minimally polymorphic ligands, gp41, CD4 and chemokine receptors, each exhibit particular problems with respect to the elicitation of sensitivity to neutralizing antibodies. The moieties involved in gp120-gp41 association are buried in the  
35 interior of the functional envelope glycoprotein spike (18, 31, 32). The CD4 binding sites is recessed, flanked by variable regions exhibiting considerable

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glycosylation (19,20). The chemokine receptor-binding site is masked by variable loops, probably V3 and V2 (20,32,33) (Figure 27c). Even in the relatively conserved HIV-1 gp120 core that has been structurally analyzed, the outer domain exhibits a variable, heavily glycosylation surface (20). Since most carbohydrate moieties may appear as "self" to the immune system, this concentrated glycosylation may reduce the potential of a large portion of the gp120 surface to serve as an immunogenic target. Thus, in addition to the neutralizing and nonneutralizing faces of gp120 previously detected by antibody competition analysis (32), the crystal structure of the gp120 core reveals a third, immunologically silent face of gp120 (Fig 6D).

Despite the potential to exert potent antiviral effects, antibodies are not able to suppress virus replication completely in infected hosts. The efficacy of the humoral immune response in limiting virus spread in vivo is compromised by at least two factors: 1) the relative resistance of primary virus isolates to neutralization; and 2) the temporal pattern with which neutralizing antibodies are generated.

Decreased neutralization sensitivity of primary HIV-1 isolates.

HIV-1 viruses that have been passaged in immortalized cell lines are typically more sensitive to neutralization by antibodies or soluble CD4 than are primary, clinical isolates (34). Although other envelope glycoprotein regions can influence this phenotype, a major determinant is the structure of the gp120 major variable loops, V1/V2 and V3 (35). Thus, replacement of the V1/V2 and V3 variable loops of a laboratory-adapted virus with those of a neutralization-resistant primary isolate creates a virus similar to the parental primary virus (35). The basis for the



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decreased sensitivity of primary HIV-1 isolates to neutralization appears to involve a decreased exposure of the relevant gp120 epitopes to soluble CD4 or antibody. This decrease is most apparent in the context  
5 of the assembled oligomeric complex (36). A likely explanation for this neutralization resistance is that the major variable loops of primary viruses assume tightly interfacing, "closed" conformations that decrease the accessibility of many gp120 epitopes to  
10 antibodies.

The temporal pattern of the antibody response to HIV-1 infection.

The noncovalent nature of the association between gp120  
15 and gp41 contributes to the lability of the functional envelope glycoprotein trimer (8,9). During natural infections, disassembled envelope glycoproteins apparently elicit most of the antibodies directed against these viral components. The interactive regions  
20 of gp120 and gp41 are particular immunogenic (37). However, since the cognate antibodies cannot bind the assembled, functional envelope glycoprotein complex, they do not exhibit neutralizing activity. Thus, although antibodies against the envelope glycoproteins  
25 typically can be detected in the sera of HIV-1-infected individuals by two-three weeks after infection, most of these antibodies lack the ability to inhibit virus infection. By the time that neutralization antibodies are efficiently elicited, HIV-1 is firmly established in  
30 the host.

Several weeks after virus infection, usually after the initial high level of viremia has subsided, neutralizing antibodies can be detected in the sera of infected  
35 animals or humans (38). These antibodies neutralize the infecting virus but often exhibit little or no activity against other strains of virus. A subset of these

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strain-restricted antibodies recognize the HIV-1 V3 loop (38). These antibodies can block chemokine receptor binding (14). Other variable gp120 elements can contribute to the epitopes recognized by the strain-restricted neutralizing antibodies. It is known, for example, that antibodies directed against the gp120 V2 loop can also exhibit neutralizing activity (39). The V2 loop-associated neutralization epitopes are typically conformation-dependent. The ability of some V2-or V3-directed antibodies to recognize more than one HIV-1 strain (39,40) suggests that these major variable loops assume a finite number of conformations. This is consistent with the functional consequences on virus entry of some changes in these variable structures (41), and with the observation that amino acid substitutions in the variable loops are not random (42). The requirement for chemokine receptor binding probably constrains V3 loop variation. The V2 loop, although dispensable for the replication of some HIV-1 viruses in culture (33), helps protect the V3 loop and the conserved epitopes near the chemokine receptor binding site from neutralizing antibodies. Thus, the V2 and V3 loops reside proximal to the chemokine receptor binding site (Fig. 27), masking more conserved gp120 elements and presenting potentially variable epitopes to the immune system.

Later in the course of HIV-1 infection of humans, antibodies capable of neutralizing a wider range of HIV-1 isolated appear (43). A subset of the broadly reactive neutralizing antibodies, found in most HIV-1 infected individuals, interferes with the binding of gp120 and CD4 (43). Human monoclonal antibodies derived from HIV-1 infected individuals have been identified that recognize the gp120 glycoproteins from a diverse range of HIV-1 isolates, that block gp120-CD4 binding, and that neutralize virus infection (44). The

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discontinuous epitopes (the so-called CD4BS epitopes) recognized by many of these human monoclonal antibodies have been characterized by mutagenic analysis (45). The gp120 residues important for antibody binding are all located within the CD4-binding pocket on gp120 (Fig. 27b), and several of the most important residues are near the opening of the deep cavity (20). Therefore, some broadly neutralizing antibodies can apparently access the more recessed elements of the CD4 binding pocket. This is consistent with the observation that the gp120-CD4 interface is as large as that of a typical antibody-antigen complex (20).

A second group of neutralizing antibodies found in a smaller number of HIV-1-infected humans is directed against the CD4-induced (CD4i) epitopes (46). The CD4i epitopes are located near conserved gp120 structures important for chemokine receptor interaction (14) (Fig. 27b). CD4 binding has been shown to cause a change in the V2 loop conformation that allows better CD4i epitope exposure (33). In the absence of CD4, the antibodies recognizing the CD4i epitopes must bypass the overlapping V2 and V3 loops (33). Indeed, as is evident in the current crystal structure (20), this is accomplished by the protrusion of the CDR3 loop of the antibody heavy chain. Antibodies against CD4i epitopes need to bind viruses before CD4 binding occurs to achieve neutralization (47). The reason is that once the envelope glycoprotein complex binds cell surface CD4, there are severe steric constraints on the binding of an antibody to the gp120 surface facing the target cell (Fig. 26).

Another fairly conserved gp120 neutralization epitope is recognized by the 2G12 antibody (48). Unlike the other characterized HIV-1 neutralizing antibodies, which recognize gp120 structures near or within the receptor-

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binding sites, the 2G12 antibody apparently binds an epitope in the outer domain (Fig. 27b). Given the variability in this outer domain, the ability of the 2G12 antibody to neutralize a fair number of HIV-1 strains (48) seems paradoxical. The marked sensitivity of 2G12 binding to alterations in gp120 glycosylation provides a clue to this puzzle. Despite the variability of the underlying primary amino acid sequence, the 2G12 antibody may recognize more conserved carbohydrate structures formed as a result of the heavy concentration of N-linked glycosylation in the gp120 outer domain. The apparent rarity with which 2G12-like antibodies are elicited attests to the success of the viral strategy of employing a heavily glycosylated outer domain surface in immune evasion.

The HIV-1 envelope glycoproteins as vaccine components.

That the human and simian immunodeficiency virus envelope glycoproteins are not ideal immunogens is an expected consequence of the immunological selective forces that drove the evolution of these viruses. The same features of the envelope glycoproteins that dictate poor immunogenicity in natural infections have hampered vaccine development. The lability of envelope glycoprotein complex has frustrated attempts to present oligomers mimicking the functional spike to the immune system. As discussed above, the disintegration of envelope glycoprotein oligomers contributes to the preferential elicitation of non-neutralizing antibodies by the newly exposed gp120 N- and C-termini. Regardless of the context in which the envelope glycoproteins are presented, the gp120 variable loops elicit the majority of neutralizing antibodies, probably due to the exposed nature of these epitopes. It is still unclear whether conserved features in the V2 and V3 variable loops exist that can be exploited in vaccine design, or whether all possible functional configurations of these variable

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structures need to be represented in a cocktail of immunogens.

5 The discontinuous gp120 structures surrounding the receptor binding sites exhibit a relatively high degree of conservation (20), in keeping with the minimal polymorphism in the host cell receptors. The CD4 binding site contributes a particularly attractive target. It appears to be accessible to antibodies, more  
10 so than the conserved elements of the chemokine receptor-binding region. A large fraction of the broadly neutralizing antibodies that eventually appear in HIV-1-infected individuals is directed against the CD4 binding site (43), indicating that ability of the  
15 human immune system to recognize this gp120 region and to generate an appropriate response. Nonetheless, these antibodies have been difficult to elicit in animals and vaccinated humans (49). The reasons for the relatively poor immunogenicity of the CD4 binding site are not yet  
20 understood, although several possibilities can be envisioned. Interdomain flexibility may disrupt the CD4BS epitopes and decrease their representation in the pool of immunogens. Masking by variable loops (19,33) and glycosylation may contribute to the recessed nature  
25 of the CD4BS epitopes which, even on the crystallized gp120 core, occupy a 20 Å deep canyon (20). Within the CD4-binding pocket, not all of the gp120 surface is conserved among HIV-1 strains. Therefore, even when elicited, some CD4BS-directed antibodies may lack the  
30 breadth and affinity to be optimal neutralization agents. While many monoclonal antibodies against the CD4 binding site exhibit reasonable potency and breadth (44), whether a polyclonal response against the envelope glycoprotein can be focused to preferentially contain  
35 these types of antibodies remains to be seen.

The conserved element near the chemokine receptor-

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binding site will be difficult target for vaccine-  
elicited antibodies. Known monoclonal antibodies to the  
CD4i epitopes must interact with virus prior to CD4  
binding if neutralization is to be achieved (47). Yet  
5 these gp120 structures are poorly exposed in the absence  
of CD4, in large part due the overlying V2 loop (33).  
This is consistent with the relative rarity with which  
these antibodies appear to be elicited in HIV-1-infected  
humans (46). Attempts to expose these structures better  
10 on gp120-based antigens seem warranted.

#### Summary

The HIV-1 envelope glycoproteins have evolved to be  
inefficient at eliciting effective antiviral antibody  
15 responses. The availability of structural information  
on the conserved HIV-1 gp120 neutralization epitopes  
should facilitate the modification of this important  
antigen and allow the rational testing of hypotheses  
regarding its poor immunogenic properties. These  
20 efforts should complement ongoing efforts to improve  
antigen presentation to the immune system and to create  
suitable animal models for the screening of vaccine  
candidates.

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### Third Series of Experiments

The entry of human immunodeficiency virus (HIV) into cells requires sequential interactions of the viral exterior envelope glycoprotein, gp120, with the CD4 glycoprotein and a chemokine receptor on the cell surface. These interactions initiate a fusion of the viral and cellular membranes. Although gp120 can elicit virus-neutralizing antibodies, HIV eludes the immune system. We have solved the X-ray crystal structure at 2.5Å resolution of an HIV-1 gp120 core complexed with a two-domain fragment of human CD4 and an antigen-binding fragment of a neutralizing antibody that blocks chemokine-receptor binding. The structure reveals a cavity-laden CD4-gp120 interface, a conserved binding site for the chemokine receptor, evidence for conformational change upon CD4 binding, the nature of a CD4-induced antibody epitope, and specific mechanisms for immune evasion. Our results provide a framework for understanding the complex biology of HIV entry into cells and will guide efforts to intervene.

### Introduction

Human immunodeficiency viruses, HIV-1 and HIV-2, and the related simian immunodeficiency viruses (SIV) cause the destruction of CD4<sup>+</sup> lymphocytes in their respective hosts, resulting in the development of acquired immunodeficiency syndrome (AIDS) (1, 2). The entry of HIV into host cells is mediated by the viral envelope glycoproteins, which are organized into oligomeric, probably trimeric, spikes displayed sparsely on the surface of the virion. These envelope complexes are anchored in the viral membrane by the gp41 transmembrane envelope glycoprotein. The surface of the spike is composed primarily of the exterior envelope glycoprotein, gp120, associated by noncovalent

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interactions with each subunit of the trimeric gp41 glycoprotein complex(3, 4.) When the gp120 sequences of different primate immunodeficiency viruses were initially compared, five variable regions (V1-V5) were identified (5). The first four variable regions form surface-exposed loops that contain disulfide bonds at their bases (6). The conserved gp120 regions form discontinuous structures important for the interaction with the gp41 ectodomain and with the viral receptors on the target cell. Both conserved and variable gp120 regions are extensively glycosylated(6). The variability and glycosylation of the gp120 surface likely modulate the immunogenicity and antigenicity of the gp120 glycoprotein, which is the major target for neutralizing antibodies elicited during natural infection (7).

Entry of primate immunodeficiency viruses into the host cell involves the binding of the gp120 envelope glycoprotein to the CD4 glycoprotein, which serves as the primary receptor. The gp120 glycoprotein binds to the most amino-terminal of the four immunoglobulin-like domains of CD4. Structures of both the N-terminal two domains (8, 9) and the entire extracellular portion of CD410 have been determined, and mutagenesis studies indicate that the CD4 structure analogous to the second complementarity-determining region (CDR2) of immunoglobulins is critical for gp120 binding(11, 12). Conserved gp120 residues important for CD4 binding have likewise been identified by mutagenesis (3, 13, 14).

CD4 binding induces conformational changes in the gp120 glycoprotein, some of which involve the exposure and/or formation of a binding site for specific chemokine receptors. These chemokine receptors, mainly CCR5 and CXCR4 for HIV, serve as obligate second receptors for virus entry (15, 16.) The gp120 third variable (V3) loop is the major determinant of chemokine receptor



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specificity (17). However, other more conserved gp120 structures that are exposed upon engagement of CD4 also appear to be involved in chemokine-receptor binding. This CD4-induced exposure is indicated by the enhanced binding of several gp120 antibodies (18, 19) which, like V3-loop antibodies, efficiently block the binding of gp120-CD4 complexes to the chemokine receptor (20). These are called the CD4-induced (CD4i) antibodies. CD4 binding may trigger additional conformational changes in the envelope glycoproteins. For example, the binding of CD4 to the envelope glycoproteins of some HIV-1 isolates induces the release or "shedding" of the gp120 protein from the complex (21), although the relevance of this process to HIV entry is uncertain.

HIV and related retroviruses belong to a class of enveloped fusogenic viruses that includes corona-, paramyxo- and orthomyxoviruses (e.g. influenza virus), all of which require post-translational cleavage for activation. The transmembrane coat proteins of these viruses (gp41 equivalents) share sequence resemblance, particularly in their N-terminal fusion peptides, and they participate directly in membrane fusion. The ectodomain of gp41 can form a coiled coil resembling that of influenza hemagglutinin HA<sub>2</sub> (23, 4, 22,) supporting the notion that this class of viruses may share some common aspects with respect to virus entry. In other respects, enveloped viruses tend to be distinctive. They use varying modes of entry (direct membrane penetration for HIV, endocytosis for influenza virus) and even otherwise closely related viruses may use individualized receptors. The exterior coat proteins (gp120 equivalents) are accordingly specialized. Thus, for example, there is no detectable similarity in sequence, nor now in structure, between the receptor binding portion of HIV and that of murine leukemia virus (23), another retrovirus. Mechanisms for

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receptor-mediated triggering of fusion may also be virus specific.

5 Because of the key role that the gp120 glycoprotein plays in receptor binding and in interactions with neutralizing antibodies, knowledge of the gp120 structure is important for understanding HIV infection and for the design of therapeutic and prophylactic strategies. Here, we report the crystal structure, at  
10 2.5 Å resolution, of an HIV-1 gp120 core bound to a two-domain fragment of the CD4 cellular receptor and to the antigen-binding fragment (Fab) of an antibody, 17b, that is directed against a CD4i epitope. A companion report relates this structure to the antigenic  
15 properties of the gp120 envelope proteins(24).

#### Structure determination

The extensive glycosylation and conformational  
20 heterogeneity associated with the HIV-1 gp120 glycoprotein recommended a crystallization strategy aimed at radical modification of the protein surface. We made truncations at termini and variable loops in various combinations with gp120 from various strains,  
25 extensively deglycosylated these gp120 variants, and produced complexes with various ligands. A theoretical analysis showed that the probability of crystal formation is greatly increased by such reduction of surface heterogeneity and trials with multiple  
30 variants(25). After screening almost twenty combinations of gp120 variants and ligands, we obtained crystals of a ternary complex composed of a truncated form of gp120, the N-terminal two domains (D1D2) of CD4, and an Fab from the human neutralizing monoclonal  
35 antibody 17b (18, 25).

The crystallized gp120 is from the HXBc2 strain of

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HIV-1. It has deletions of 52 and 19 residues from the N- and C- termini, respectively; Gly-Ala-Gly tripeptide substitutions for 67 V1/V2-loop residues and 32 V3-loop residues; and the removal of all sugar groups beyond the linkages between the two core N-acetylglucosamine residues. This deglycosylated core gp120 eliminates over 90% of the carbohydrate but retains over 80% of the non-variable-loop protein. Its capacity to interact with CD4 and relevant antibodies is preserved at or near wild-type levels<sup>26</sup>. The crystals are of space group P222<sub>1</sub> (a=71.6, b=88.1, c=196.7Å) with one ternary complex and 60% solvent in the crystallographic asymmetric unit.

The ternary structure was solved by a combination of molecular replacement, isomorphous replacement, and density modification techniques. It has been refined to an R-value of 21.0% (5-2.5 Å data > 2σ, R-free=30.3%). The final model, composed of 7877 atoms comprises residues 90-396 and 410-492 of gp120 (excepting loop substitutions), residues 1-181 of CD4, and residues 1-213 of the light chain and 1-229 of the heavy chain of the 17b monoclonal antibody. In addition, 11 N-acetylglucosamine and 4 fucose residues, and 602 water molecules have been placed. The overall structure of the complex of gp120 with D1D2 of CD4 and Fab 17b is as depicted in Fig. 28.

#### Structure of gp120

The deglycosylated core of gp120 as dissected from the ternary complex approximates a prolate ellipsoid with dimensions of 50 x 50 x 25Å, although its overall profile is more heart-shaped than circular. Its backbone structure is shown in Figs. 29a & c in an orientation precisely perpendicular to that in Fig. 28 (Fig. 31e gives a mutually perpendicular view). This

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core gp120 comprises 25 b strands, 5 a helices and 10 defined loop segments, all organized with the topology shown in Fig. 29b. Specific spans of structural elements are given in Fig. 29d. The structure confirms  
5 the chemically determined disulfide bridge assignments (6; Fig. 29c). The polypeptide chain of gp120 is folded into two major domains plus certain excursions that emanate from this body. The inner domain (inner with respect to the N- and C-termini) features a two-helix,  
10 two-strand bundle with a small five-stranded  $\beta$ -sandwich at its termini-proximal end and a projection at the distal end from which the V1/V2 stem emanates. The outer domain is a stacked double barrel that lies alongside the inner domain such that the outer barrel  
15 and inner bundle axes are approximately parallel.

The proximal barrel of the outer-domain stack is composed from a 6-stranded, mixed-directional  $\beta$ -sheet that is twisted to embrace helix  $\alpha 2$  as a 7th barrel  
20 stave. The distal barrel of the stack is a 7-stranded antiparallel  $\beta$  barrel. The two barrels share one contiguous hydrophobic core, and the staves also continue from one barrel to the next except at the domain interface. This interruption is centered at a  
25 side between barrels where the chain enters the outer domain with loop  $\lambda B$  insinuated as a tongue between strands  $\beta 16$  and  $\beta 23$ . The extended segment just preceding  $\lambda B$  is like an 8th stave of the distal barrel, but it is slightly out of reach for hydrogen bonding  
30 with its  $\beta 16$  and  $\beta 19$  neighbors. The chain returns to complete the inner domain after  $\beta 24$ .

The proximal end of the outer domain includes variable loops V4 and V5 and loops  $\lambda D$  and  $\lambda E$ , which are variable  
35 in sequence as well. Loop  $\lambda C$  is also at this end, close in space to loop  $\lambda A$  of the inner domain, although by topology it is at the other end of this domain. The

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distal end does include the stem of the excised variable loop V3 and also an excursion via loop  $\lambda F$  into a  $\beta$  hairpin,  $\beta 20$ - $\beta 21$ , which in turn hydrogen bonds with the V1/V2 stem emanating from the inner domain. This completes an antiparallel, 4-stranded "bridging sheet" that stands as a peculiar minidomain in contact with, but distinct from, the inner and outer domains as well as the excised V1/V2 domain. This bridging sheet also participates in the separated interactions of gp120 with both CD4 and the 17b antibody (Fig. 28 and below). One further excursion from the body of the outer domain produces strand  $\beta 15$  and helix  $\alpha 3$ , which are also important in CD4 binding.

Taken as a whole the structure of gp120 seen here is novel. Moreover, our domain-level searches have failed to reveal similarity of the inner domain to any known atomic structures, although the missing terminal segments might conceal relationships. We do, however, find a fragmentary similarity for portions of the outer domain with known structures. In particular, part of the protomer of FabA dehydrase (27) is like part of the proximal barrel, and dUTP pyrophosphatase (28) has elements in common with both barrels of the outer domain. In each case the superimposable fraction is limited. For FabA, 45 of its 171 C-alpha atoms superimpose on five segments, but the rest are topologically unrelated. For dUTPase, 41 of its 152 C-alpha atoms appropriately capture 8 of the 15 segments in the outer domain body, but there is no helix corresponding to alpha-2 and the placements of termini are not comparable. Interestingly, several viruses related to HIV encode dUTPases; however, we have not found sequence evidence to support a possible role in coat protein evolution.

This structure of core gp120 should be a prototype for

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the class. As shown in the structure-based alignment of representative sequences (Fig. 29d), there is substantial conservation despite the noted variability among HIV strains. Thus, even an HIV-2 sequence is 35% identical with that of the HXBc2 strain expressed in this crystallized construct, and the identity level rises to 77% and 51%, respectively, for the more closely related HIV-1 clade C and clade O representatives. The inner domain is appreciably more conserved than the outer domain with 86%, 72% and 45% identity for the respective C, O and HIV-2 comparisons. Variability correlates with the degree of solvent exposure of residues (Fig. 29d), in keeping with the conservation of hydrophobic cores. The seven disulfide bridges retained in core gp120 are absolutely conserved and mostly buried (Fig. 29c). Glycosylation sites are all surface exposed and are conserved above average (Fig. 29d). The previously identified HIV variable segments(5) are all on loops connecting elements of secondary structure, and loops  $\lambda$ D and  $\lambda$ E are also especially variable. Indeed,  $\lambda$ E is more variable than V5 in light of current sequence data. These loops are also relatively mobile as reflected in high B factors or disorder, as in V4. Interestingly, variable segments in the outer domain, including the exposed face of  $\alpha$ 2, appear to arise from neutral mutation rather than selective pressure since they are on non-immunogenic surfaces, presumably masked by glycosylation.

### 30 CD4-gp120 interaction

CD4 is bound into a depression formed at the interface of the outer domain with the inner domain and the bridging sheet of gp120 (Figs. 30a). This interaction buries a total of 742  $\text{\AA}^2$  from CD4 and 802  $\text{\AA}^2$  from gp120. The surface areas that are actually in contact are considerably smaller (Fig. 30d) because an unusual

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mismatch in surface topography creates large cavities that are occluded in the interface, as described below. There is, however, a general complementarity in electrostatic potential at the surfaces of contact, although the match is imprecise in this respect as well. The focus of CD4 positivity is displaced from the center of greatest negativity on gp120 (Fig. 30c). The binding site is devoid of carbohydrate (Fig. 30g). The structure of CD4 in this complex differs only locally from that in free D1D2 structures and at only a few places: residues 17-20 at the poorly ordered CDR1-like loop and residues 41,42,47,49 and 60, which are at or near the contact site and have low B factors in the gp120-bound state.

Direct interatomic contacts are made between 22 CD4 residues and 26 gp120 amino-acid residues. These include 219 van der Waals contacts and 12 hydrogen bonds. Residues in contact are concentrated in the span from 25 to 64 of CD4, but they are distributed over six segments of gp120 (Figs. 29d & 30i): 1 residue from the V1/V2 stem, loop LD, the beta-15-alpha-3 excursion, the beta-20-beta-21 hairpin, strand beta-23 and the beta-24-alpha-5 connection. These interactions are compatible with previous analyses of mutational data on both CD4(11, 12, 29) and gp120(3, 13, 14). Other groups are also involved, including some at gp120 sites that have not been tested, but residues identified as critical for binding do indeed interact with one another (Fig. 30e). Most importantly, Phe 43 and Arg 59 of CD4 make multiple contacts centered on residues Asp 368, Glu 370 and Trp 427 of gp120, which are all conserved among primate immunodeficiency viruses. In fact, 63% of all interatomic contacts come from one span (40-48) in C'C" of CD4, and Phe 43 alone accounts for 23% of the total. Similarly, with respect to gp120, the spans of 365-371 and 425-430 contribute 57% of the total. Of the three

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CD4 lysine residues implicated in binding (residues 29, 35 & 46), only Lys 29 makes a direct ionic hydrogen bond, and while Asp 457 of gp120 is near to these electropositive groups (Figs. 30e & i) it does not make  
5 hydrogen bonds.

Several gp120 residues that are covered by CD4 are variable in sequence. This variation is accommodated in part by the large interfacial cavity (Fig. 30e). The  
10 gp120 residues in contact with this water-filled cavity are especially variable (Fig. 30g). Moreover, half of the gp120 residues that make contacts with CD4 do so only through main-chain atoms (including C $\beta$ ) of gp120, and 60% of CD4 contacts are made by gp120 main-chain  
15 atoms (Fig. 30f). Included among these are 5 of the 12 hydrogen bonds in the interface. One such contributing element is an antiparallel  $\beta$ -sheet alignment of CD4 strand C" with gp120 strand beta-15 (Figs. 30a & i).

20 Atomic details of the interaction are particularly intricate and unusual for the contacts made between gp120 and the mutationally critical CD4 residues Phe 43 and Arg 59 (Fig. 30j). Arg 59 interacts with Asp 368 and Val 430. The carboxylate group of Asp 368 makes  
25 double hydrogen bonds with the guanidinium N $\eta$  atoms of Arg 59, but it also hydrogen bonds back to the backbone NH group of residue 44 and it appears to be optimally positioned to receive a CH...O hydrogen bond (3.20 Å) from the Phe 43 ring. Phe 43 interacts with residues  
30 Glu 370, Ile 371, Asn 425, Met 426, Trp 427 and Gly 473 as well as Asp 368, but only the contacts with Ile 371 have a conventional hydrophobic character. Those to 425-427 and 473, including Trp 427, are only to backbone atoms. A surprisingly large fraction of the Phe 43  
35 contacts (28%) are to polar groups. The phenyl group is stacked on the carboxylate group of Glu 370, and there are contacts with the carbonyl oxygen atoms of residues



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425, 426 and 473 and the NH group of Trp 427. Indeed, at a distance of 3.10 Å, the phenyl contact with O 425 is a second candidate CH...O hydrogen bond. Asp 368 and Glu 370 have their carboxylate groups close together (3.54 Å) and they are, of course, buried in the complex. Even for gp120 excised from the complex, their fractional surface accessibilities are only 44% and 14%, respectively. Glu 370 may therefore be protonated. Perhaps the most extraordinary aspect of this site is the large cavity beyond C $\alpha$  of Phe 43 (Figs. 30b & h, and below).

#### Interfacial cavities

Analysis of the solvent accessible surface of the ternary complex reveals a number of topologically interior surfaces or cavities. Two of these, both at the gp120-CD4 interface, are unusually large. The larger (279 Å<sup>3</sup>) is formed at the interface between the slightly concave middle of the CC'C" portion of the CD4 sheet, and a groove on gp120 where beta-23 and beta-24 are indented relative to beta-15 and the  $\lambda$ D loop (Fig. 30e). The second is from a pocket in the gp120 surface that is plugged by Phe 43 from CD4 (152 Å<sup>3</sup>). This pocket is itself at the interface between the inner and outer domains of gp120 (Fig. 30h). Several other smaller cavities are also wedged at the interface between the two gp120 domains.

The larger cavity is lined by mostly hydrophilic residues, half derived from gp120 and half from CD4. It is not deeply buried; while formally a cavity in the crystal structure, minor changes in sidechain orientation would make it solvent accessible. The observed electron density and predicted hydrogen bonding are consistent with at least 8 water molecules in the cavity. Residues from gp120 that actually line the



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The center of the cavity is dominated by a large piece of spherical density, which is over 4 Å from any protein atom (Fig. 30b). The size, shape and predicted hydrogen bonding of this density is inconsistent with those expected for water, isopropanol, ethylene glycol, or any of the other major crystallization components. We have been unable to identify the source of this density.

Residues that line the Phe 43 cavity (side chains of Trp 112, Val 255, Thr 257, Glu 370, Phe 382, Tyr 384, Trp 427 and Met 475; main chains of 255-257 and 375-377) are primarily hydrophobic. They are also highly conserved, as much so as the buried gp120 hydrophobic core. Despite a lack of steric hindrance, almost no substitutions to larger residues are found. Given the frequency of gp120 sequence divergence, such conservation strongly implies functional significance. Indeed, although residues that line this cavity provide little direct contact to CD4, they do nevertheless affect the gp120-CD4 interaction. Thus, mutations at Thr 257 (no contacts) and Trp 427 (only main-chain contacts) can substantially reduce binding. Changes in cavity-lining residues also affect the binding of antibodies directed against the CD4 binding site. In addition, many of the residues that line the cavity interact with elements of the chemokine receptor binding region (see below). It may be that the Phe 43 cavity and the other interdomain cavities form as a consequence of a CD4-induced conformational change (see below).

Despite this unusual cavity-laden interface between gp120 and CD4 interface, we believe that this structure reflects the true character of the interaction. Core gp120 binds CD4 with essentially the same affinity(26) and residues identified as critical by mutational analysis on both components are indeed at the focus of contact in the structure. In any case, the missing

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loops and termini could not conceivably have a role in filling these cavities.

#### Antibody interface

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The 17b antibody is a broadly neutralizing human monoclonal isolated from the blood of an HIV-infected individual. It binds to a CD4-induced (CD4i) gp120 epitope that overlaps the chemokine receptor-binding site(20).

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Relative to other antibody-antigen pairs (Fig. 31a-c), the interface between Fab 17b and core gp120 in the ternary complex involves a small area of interaction. The solvent accessible area excluded upon binding is only 455 Å<sup>2</sup> from gp120 and 445 Å<sup>2</sup> from 17b, which is largely from the heavy chain (371Å<sup>2</sup>). The long (15 residue) complementarity-determining region 3 (CDR3) of the heavy chain dominates, but the heavy-chain CDR2 and the light-chain CDR3 also contribute. Overall, the 17b contact surface is very acidic (3 Asp, 3 Glu, no Arg or Lys) although hydrophobic contacts (notably a cis proline and tryptophan from the light chain) predominate at the center.

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On gp120, the 17b epitope lies across the base of the four-stranded bridging sheet (Fig. 31c & e). All four strands make substantial contact with 17b, suggesting that the integrity of the bridging sheet is necessary for 17b binding. The gp120 surface that contacts 17b consists of a hydrophobic center surrounded by a highly basic periphery (3 Lys, 1 Arg, and no Asp or Glu) (Fig. 31d). Although this basic gp120 surface complements the acidic 17b surface, only one salt bridge is observed (between Arg 419 of gp120 and Glu 106 of the 17b heavy chain). The rest of the specific contacts occur between hydrophobic and polar residues. Thus, the interaction

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between 17b and gp120 involves a hydrophobic central region flanked on the periphery by charged regions, predominately acidic on 17b and basic on gp120. There are no direct CD4-17b contacts and none of the gp120 residues contacts both 17b and CD4. Rather, CD4 binds on the opposite face of the bridging sheet, providing specific contacts that appear to stabilize its conformation (Fig. 30i and 30j) and may explain in part the CD4-induction of 17b binding.

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The 17b epitope is well conserved among HIV-1 isolates. Of the 18 residues that show loss in solvent accessible surface upon contact with 17b, 12 residues (67%) are conserved among all HIV-1 viruses. By contrast, only 19 of the 37 gp120 residues (51%) that show loss of solvent accessible surface upon CD4 binding are similarly conserved. CD4i epitopes tend to be masked from immune surveillance by the adjacent V2 and V3 loops (see accompanying paper). Indeed, in the complex structure, a large gap is seen between gp120 and tips of the light-chain CDR1 and CDR2 loops. Pointing directly at this gap is the base of the V3 loop. In intact gp120, the variable loops may need to be bypassed for access to the conserved structures in the bridging sheet. The 17b epitope may be further protected from the immune system by a CD4-induced conformational change (see below).

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#### Chemokine receptor site

The site of interaction with the chemokine receptor CCR5 overlaps with the 17b epitope(30). Both are induced upon CD4 binding and both involve highly conserved residues. By mutational analysis, the basic and polar gp120 residues (Lys 121, Arg 419, Lys 421, Gln 422) that contact the 17b heavy chain also are important for CCR5 interaction(30). The hydrophobic and acidic surface of the 17b heavy chain may mimic the tyrosine-rich, acidic

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N-terminal region of CCR5, which is important for gp120 binding and HIV-1 entry (31, 32). Geometrically, this site is directed at the cellular membrane when gp120 is engaged by CD4. Electrostatic interactions between the  
5 basic surface of the bridging sheet and the acidic chemokine receptor (and possibly the acid headgroups in the target membrane) could drive conformational changes related to virus entry.

#### 10 Oligomer and gp41 interactions

Although monomeric in isolation, gp120 likely exists as a trimeric complex with gp41 on the virion surface. The large electroneutral surface on the inner domain (Fig.  
15 30c) is the probable site of trimer packing based on its lack of glycosylation, its conservation in sequence, the location of CD4 and CCR5 binding sites, and the immune response to this region. These points are elaborated in the accompanying paper and a model is presented(24).

20

A large body of mutagenic and antibody-binding analyses suggest that the N- and C-termini of full-length gp120 are the most important regions for interaction with the gp41 glycoprotein (33, 34). From these analyses, we  
25 expect that gp41 interactive regions will extend away from core gp120 toward the viral membrane, and that the conserved, electroneutral surface is occluded in the oligomer/gp41 interface. A similar arrangement is seen in influenza hemagglutinin, where the extended N- and  
30 C-termini of HA<sub>1</sub> interact with the HA<sub>2</sub> transmembrane protein (35).

#### Conformational change in core gp120

35 There is abundant evidence to suggest that CD4 binding induces a conformational change in gp120. Much of this evidence, however, derives from intact gp120 with

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variable loops in place or from the oligomeric gp120:gp41 complex. The ternary complex structure provides clues to conformational changes within core gp120 itself. (Although 17b binding could contribute to the gp120 conformation observed in the crystal, the CD4 contacts are much more extensive and multifaceted than those of 17b. These observations argue that CD4 binding plays the major role in the formation of the observed gp120 structure.)

Were the conformation of gp120 seen here preserved in the absence of CD4, the Phe 43 cavity (now a pocket) would present a perplexing structural dilemma. As discussed above, the cavity-lining residues have few structural restrictions, with ample room for larger substitutions into the cavity, yet these residues are highly conserved and inexplicably hydrophobic if exposed in a pocket. This pocket structure is in turn intimately connected to the bridging sheet, itself peculiar in absence of CD4. Thus, for example, the backbone amide of bridging-sheet residue 425 is hydrogen-bonded to Glu 370, a critical CD4 contact residue (Fig. 30j); Ile 424 makes extensive hydrophobic contacts with Phe 382, which lines the pocket from the outer domain; and Trp 427 packs perpendicular to Trp 112, which lines the pocket from the inner domain (Fig. 30b). NE of Trp 427 is delicately poised for hydrogen-bonding with the  $\pi$ -electrons of the indole ring of Trp 112. Structures such as these would necessarily be very sensitive to orientational shifts between the inner and outer domains.

The characteristics of 17b binding to core gp120 provide additional evidence for a CD4-induced conformational change. We do not observe detectable binding of Fab 17b to core gp120 unless CD4 is present, but then the ternary complex is stable in gel filtration. Since

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there are no direct CD4-17b contacts in the structure, the effect of CD4 must be to stabilize the bridging-sheet minidomain to which 17b binds. This result is compatible with the binding properties of 17b and other CD4i antibodies to full-length gp120(18) (see accompanying paper), but it shows that the conformational change is not limited to an unmasking of the antibody epitope by CD4-induced of the V2 loop, as initially thought(36). The ability of the 17b antibody to bind full-length gp120 in the absence of CD4, albeit at a lower level, implies that structural elements required for 17b binding can be accessed in the absence of CD4. If we assume that 17b binds in the same way to both full-length and core gp120, as shown by the concordance between the structural contacts (Fig. 31) and epitope mapping data, this suggests that alternative conformations are in a kinetically accessible equilibrium in native gp120.

A further indication that core gp120 may differ in the absence of CD4 comes from comparison with theory. When applied to the many known sequence variants of gp120, the evolutionary algorithm of PHD37 gives secondary-structure predictions with 90% estimated reliability for roughly 45% of the core gp120 sequence. Compared to our structure, it is accurate except at three places where it is markedly wrong (four consecutive residues with reliability index greater than 90%). All of these are at the Phe 43 cavity or in contacts with CD4: loop  $\lambda$ B, strand  $\beta$ 15, and the segment of  $\beta$ 20 into the turn to  $\beta$ 21. (Fig. 30h). Most significantly, the latter segment (residues 422-429) entering the bridging sheet is predicted to be helical. Indeed, residues 427-428 at the  $\beta$ 20- $\beta$ 21 turn do have helical character. We also note that CD4 binds efficiently to a gp120 derivative with both  $\beta$ 2 and  $\beta$ 3 truncated(38). Since the bridging sheet is most likely



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not stable in the absence of half its strands, CD4 binding must possess the ability to properly orient strands  $\beta 20$  and  $\beta 21$  from a very different prior conformation.

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The Phe 43 cavity is at the nexus of the CD4 interface, between the inner domain, the outer domain, and the bridging sheet. As such, Phe 43 itself seems to serve as a keystone without which the structure might collapse. If so, to what state and, in reverse, how does CD4 binding lead to the state seen in this ternary complex? Certainly, it is clear that CD4-gp120 binding kinetics are complex(39), and microcalorimetric analysis reveals unusually large  $\Delta H$  and compensating T $\Delta S$  values for soluble CD4 binding to gp120 (M. L. Doyle, personal communication). These exceptional CD4-binding thermodynamics imply a large conformational change and are similar for both full-length and core gp120, which further supports the relevance of the structural observations on core gp120. We imagine that CD4 sees gp120 as an uneven equilibrium of conformational states, makes initial contact through electrostatic interactions (Fig. 30c), stabilizes a nascent complex state, and inserts the Phe 43 to induce formation of the Phe 43 cavity.

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#### Viral evasion of immune surveillance

Analysis of the antigenic structure of gp120 shows that most of the envelope protein surface is hidden from humoral immune responses by glycosylation and oligomeric occlusion (accompanying paper). Most broadly neutralizing antibodies generally access only two surfaces, one which overlaps the CD4 binding site (shielded by the V1/V2 loop) and the other which overlaps the chemokine receptor binding site (shielded by the V3 loop). Conformational changes in core gp120

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provide additional mechanisms for evasion from immune surveillance. In the case of the CD4-binding surface, which contains a high proportion of mainchain atoms in the complex (Fig. 30f), the conformation without CD4 bound may expose underlying sidechain variability (Fig. 30g). Escape may also be provided by the recessed nature of the binding pocket (steric occlusion) (Fig. 30a) and by a topographical surface mismatch, which encloses a variational island or "anti-hot spot" (described above, Fig. 30d). Similar mechanisms may be found in the chemokine receptor region: conformational change may hide the conserved epitope (unformed prior to CD4 binding); steric occlusion may take place between the CD4 anchored viral spike and the proximal target membrane; and an "anti-hot spot" equivalent may camouflage chemokine-receptor binding residues on the V3 loop in surrounding variability. Some of the defenses used to elude antibody-based responses may also help HIV avoid cellular immunity. Understanding the specific gp120 mechanisms of immune evasion may be prerequisite to the design of effective prophylaxis.

#### Mechanistic implications for virus entry

During virus entry, the HIV surface proteins function to fuse the viral membrane with the target cell membrane. The gp120 glycoprotein plays roles crucial to the control and initiation of fusion. One set of roles concerns positioning: locating a cell capable of productive viral infection, anchoring the virus to the cell surface, and orienting the viral spike next to the target membrane. Another set concerns timing: holding the gp41 in a metastable conformation and triggering the coordinate release of the three N-terminal fusion peptides of the trimeric gp41. While it is clear that this is a complex multi-conformational process, the simplicity of the system, composed only of two

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membranes, the viral oligomer, and two host receptors, raises the possibility that we may be able to understand the entire mechanism. Crystallography has now provided two snapshots: an intermediate state in which gp120 is bound to CD4, described herein; and a probably final, "fusion-active" state of the gp41 ectodomain (40,41). Although precise structural information is lacking for other intermediates, the vast biochemical data concerning the membrane fusion process mediated by the HIV-1 envelope glycoproteins allow us to extend our understanding from these two states.

The entry process is initiated by the binding of HIV-1 to the cellular receptor CD4 (Fig. 32, step 1). Although the extracellular portion of CD4 has some segmental flexibility, this binding roughly orients the viral spike. This orientation can be simulated by an alignment of the D1D2 CD4 in the ternary complex with the previously solved structure of the four-domain, entire extracellular portion of CD4(10). Such alignment orients the N- and C- termini of core gp120 towards the viral membrane, while the 17b epitope/chemokine receptor-binding site on the gp120 surface faces the target cell membrane. Such an orientation is consistent with the proposed oligomeric structure and gp41-interactive surfaces described above.

CD4 binding also induces conformational changes in gp120, which result in the creation of a metastable oligomer. Although some of the more flexible gp120 regions and gp41 are missing, the structure of the core gp120-CD4 complex presented here describes this state in atomic detail. CD4 binding results in movement of the V2 loop, which numerous experiments suggest partially occludes the V3 loop and CD4i epitopes (18, 36). It also creates, or at least stabilizes, the bridging sheet on which these epitopes are located (described above for

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the core). In addition, CD4 binding results in changes in the conformation of the V3 region, with the tip of the loop becoming more accessible, as judged by enhanced proteolytic susceptibility and altered exposure of V3 epitopes(19). The V3 loop together with the uncovered epitopes comprise the chemokine-receptor binding site. Thus, CD4 binding not only orients the gp120 surface implicated in chemokine receptor binding to face the target cell, but it also forms and exposes the site itself. We note that these changes may all result from a single, concerted shift in the relative orientation of the inner and outer domains. This conformational shift may alter the orientation of the N- and C- termini, at the proximal end of the inner domain, perhaps partially destabilizing the oligomeric gp120/gp41 interface(21). Such a shift would also alter the relative placement of the V1/V2 stem (in the CD4i site), which emanates from the inner domain, and the V3 loop, which emanates from the outer domain. Interestingly, mutations that permit an adaptation of HIV-1 to CD4-independent entry using CXCR4 involve sequence changes in both the V1/V2 stem and the V3 loop(42).

The next step in HIV-1 entry is the interaction of the gp120-CD4 complex with the chemokine receptor (Fig. 32, step 2). Although interactions between CD4 and chemokine receptor may occur, mutagenic analyses (H. Choe and J. Sodroski, unpublished observations) and the known examples of CD4-independent virus entry or chemokine-receptor binding suggest that direct gp120 contacts dominate in the interaction with the chemokine receptor. Since most of the chemokine receptor is encased in the host membrane, binding would necessarily move the gp120 bridging sheet close to the target membrane. This movement requires CD4 flexibility since the initial HIV binding at the N-terminal D1 domains probably occurs above the glycocalyx. Reducing

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flexibility at the D2-D3 juncture or at the D4-membrane juncture of CD4 has been shown to block HIV-1 entry (10, 43).

5 Chemokine-receptor binding is believed to trigger additional conformational changes in the HIV-1 envelope glycoprotein trimer which lead to exposure of the gp41 ectodomain. Presumably, a signal is transmitted from the cell-associated distal end of gp120 to elements of  
10 the inner domain that are likely to be involved in gp120-gp41 or gp120-gp120 association on the trimer. Although further inter-domain shifts may occur in core gp120 after chemokine-receptor binding, the geometrically specific contacts that support the  
15 bridging sheet make it unlikely that another shift could occur without destabilizing this important component of the chemokine-receptor binding site. Since the high affinity of interaction makes it likely that both CD4 and chemokine receptor remain bound to gp120 during  
20 fusion, we expect that additional conformational changes probably occur between neighboring gp120 protomers in the oligomeric complex. Perhaps the chemokine receptor triggers gp41 exposure by prising gp120 protomers away from the trimer axis thus exerting a torque on the  
25 gp120-gp41 interface. In this regard it is interesting that several of the substitutions that affect chemokine-receptor binding in the context of monomeric gp120 appear to induce gp120 dissociation in an oligomeric context(30).

30 The structure of the gp120/CD4/17b antibody ternary complex described here reveals some of the molecular aspects of HIV-1 entry, including the atomic structure of gp120, the explicit interactions with CD4, and the  
35 conserved site of binding for the chemokine receptor. Still unknown are details of the apo state of core gp120, the oligomeric structure, the interaction with

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the chemokine receptor, the conformational changes that trigger the reorganization of the gp41 ectodomain and the structural basis for insertion of the fusion peptide of gp41 into the target membrane. Further understanding  
5 will require snapshots of other intermediates. The conformational complexity and observed intricate domain associations of gp120, like those of reverse transcriptase(44), the other large HIV translation product, may reflect genome restrictions at the protein  
10 level akin to those that lead to overlapping reading frames at the transcription level. Multiply protected infection machinery is contained in these condensed intricacies. Its mechanisms frustrate host defenses; understanding them may inspire medical intervention.

15

#### Methods

Protein production, crystallization, and data collection. The two-domain CD4 (D1D2, residues 1-182)  
20 was produced in Chinese hamster ovarian cells(8), the monoclonal antibody 17b in an Epstein-Barr virus immortalized B-cell clone isolated from an HIV-1 infected individual and fused with a murine B-cell fusion partner(18), and the core gp120 from Drosophila  
25 Schneider 2 lines under control of an inducible metallothionein promoter (20). The various biochemical manipulations (e.g. deglycosylation for the gp120 and papain digestion to produced the Fab 17b), protein purification, and ternary complex crystallization are  
30 described elsewhere(25). The best crystals were small needles of cross-section only 30-40  $\mu\text{m}$ . These were crosslinked with vapor diffusion glutaraldehyde treatment (C. J. Lusty, personal communication), equilibrated with cryoprotectant containing stabilizer  
35 (10% ethylene glycol with 10.5% monomethyl-PEG 5,000, 10% isopropanol, 50 mM NaCl, 100 mM Citrate/HEPES buffer pH 6.3), transferred into immiscible oil (Paratone-N;

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Exxon), suspended in a small ethylene loop at the end of a mounting pin, and flash-frozen in a cryostat nitrogen stream at 100 K .

5     Diffraction data were collected at beamline X4A, Brookhaven National Laboratory, using phosphor image plates and a Fuji BAS2000 scanner. To avoid overlap problems from the relatively high mosaicity ( $\sim 1.0^\circ$ ),  
10     oscillation data were collected using a rotation axis that was off-set at least  $30^\circ$  from the  $197\text{\AA}$  c axis. Although crystals initially diffracted to Bragg spacing of greater than  $2\text{\AA}$ ,  $\beta$  axis mosaicity and substantial radiation damage despite cryogenic cooling reduced the overall resolution to  $\sim 2.5\text{\AA}$ . Data processing and  
15     reduction were performed using DENZO and SCALEPACK(45) (Table 1).

Structure determination and refinement. To locate the position of the Fab 17b in the ternary complex crystals,  
20     rotational searches with 52 different Fab models were made with the program MERLOT (P. M. Fitzgerald). The Fabs were aligned by superposition of their variable domains to allow comparison of rotational solutions. Even though four models showed greater than 10%  
25     discrimination between highest and second highest solutions, no consistent rotational solution was found. Discrimination between correct and incorrect solutions was achieved by using confirmatory searches with the variable portion of the Fab. This was successful with  
30     only one model, molecule B of 1hil. Rigid body refinement of the 1hil solution (XPLOR(46)), allowing each immunoglobulin domain to move independently, produced a Patterson correlation of 24.9%. To locate the position of the two-domain CD4, each of the top 100  
35     possible rotational solutions with each of three different CD4 models (1cdi, 1cdh, 3cd4), were searched for a distinctive translation solution (AMoRe; J.

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Navaza). The translation searches used the rigid body refined Fab as a partial structure to help discriminate the correct solution. Two distinctive solutions were found: the 25th rotational solution of 3cd4 gave a translation correlation of 0.171 (verses 0.128 for the second highest translation solution), and the 61st rotational solution of 1cdh gave 0.149 (verses 0.140). These two solutions were virtually identical. Rigid body refinement in XPLOR(46) gave a Patterson correlation of 7.9% for the CD4 alone and 32.4% for the Fab and CD4. All molecular replacement and rigid body refinements used 8-4Å data.

To provide additional phasing, crystals were soaked in over 20 different heavy atom solutions and screened for isomorphous replacement using the statistical  $\langle\chi\rangle^2$  test in SCALEPACK(45). Derivatives were identified from two heavy atom compounds : 10 mM K3IrCl6 (10 hr equilibration in heavy atom containing cryoprotectant stabilizer; 2.8Å) and 5 mM K2OsCl6 (24 hr soak; 3.5Å). Isomorphism was found to be highest between these heavy atom data sets and a native data set collected at pH 7.0 (cryoprotectant stabilizer buffered with 50 mM BisTris pH 7.0). Heavy atom sites were identified by difference Fourier analysis using the molecular replacement phases, and phasing parameters were refined with MLPHARE (in the CCP4 suite of crystallographic programs). The K3IrCl6 derivative was modeled as 9 partially occupied sites; two sites of occupancy 0.158 and 0.142, and 7 of less than 0.07. While relatively isomorphous, poor data quality (Rsym of greater than 20% past 3.0Å) combined with relatively small isomorphous differences (Riso of 12.0%) reduced the quality of phasing. In contrast, the K2OsCl6 derivative had an Riso of 15.6%, but was only isomorphous to roughly 5Å. It was modeled as 4 sites of occupancy 0.321, 0.207, 0.194 and 0.128, with the highest site at the same position as the second highest



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site from  $K_3IrCl_6$ .

The initial combination of model and isomorphous replacement phasing did not produce readily interpretable density for gp120. In order to monitor efforts at phase improvement, we devised an objective assay of density quality that used correlations in a region internal to domain 1 of CD4 between the experimental electron density and the calculated model density (CD4 as positioned by molecular replacement and rigid body refinement). Refinement of heavy atom positions improved this correlation, and provided a starting point for phase improvement, primarily using real-space modification techniques (Table 1). These techniques included automatic concatenation of the unmodeled density (with the program PRISM; D. Agard), reciprocal-space averaging of the PRISM modeled density and real-space model subtraction (implemented using the XPLOR(46) shell language), application of real-space constraints such as solvent flattening, histogram matching and negative density truncation (with the program DM (in the CCP4 suite of crystallographic programs), and real-space combinatorial addition of the various experimental density maps (with the program MAPMAN; T.A. Jones). The combinatorial use of these techniques generated greatly improved electron density maps.

At this point, most of the carbon alpha backbone could be modeled (with the program O<sup>47</sup>) defining the secondary structure. Computer aided sequence alignment (slider routine in O) and secondary structure prediction (PHD37) helped to position the amino acid sequence leaving only regions around the N-terminus (residues 79-100 and residues 215-245), the V1/V2 loop, and the V4 loop uncertain. Iterative rounds of building with O, simulated annealing and positional refinement with

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XPLOR(46), and addition of ordered solvent clarified the trace.

Structure analysis. Deviations of the CD4 structure in  
5 the complex from the free state were measured by the  
procedure of Wu et al.(10). Deviations were taken as  
significant when the root mean square (rms) residue  
deviation was greater than the overall value and also  
10 more than 0.5Å greater than variation among the free  
structures. Interatomic contacts were defined as in Zhu  
et. al.(48). Structural alignments were made by visual  
comparison of the SCOP databas, and automatic searches  
were performed with PrISM (A.-S. Yang and B. Honig).

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**Table 1. Structure solution****Data Collection:**

	Native	K <sub>3</sub> IrCl <sub>6</sub>	K <sub>2</sub> OsCl <sub>6</sub>
Resolution limits (Å)	20-2.5	20-2.8	20-3.5
Total observations	113,966	76,739	25,821
Unique Observations	37,724	28,599	11,982
Rsym (%)†	9.3 (24.7)	11.5 (20.2)	14.3 (18.2)
Data coverage (%)*	86.0 (62.8)	90.8 (82.9)	72.5 (62.5)

**Molecular Replacement:**

	Fab	CD4	Fab+CD4
Model	1hil	3cd4/1cdh	1hil+ 1cdh
Scattering (%)‡	43	18	61
Rigid-body correlation#	0.249	0.079	0.325

**Generation of experimental electron density:**

Phasing Procedure	Correlation coefficient ‡
Molecular replacement (MR)	-0.02
Multiple isomorphous replacement (MIR)	0.34
Phase combination:	
MIR + MR	0.60
+ density modification	0.66
+ density modification + subtraction	0.69
Density modelling (concatenation):	
MIR + MR	0.65
+ density modification	0.68
+ density modification + subtraction	0.71
Combination map addition:	0.73

**Refinement Statistics:**

R-factors (10-2.5 Å):			
Data cutoff (σ)	0	2	4
R <sub>crystal</sub> (R <sub>free</sub> ) (%)	24.9 (32.8)	22.2 (30.7)	21.2 (29.2)
Data completeness (%)	85.8	77.3	66.4

**Geometric parameters (rms):**

Bond length (Å)	0.007
Bond angle (°)	1.59°

B-factors:	average	rms bond	rms angle
mainchain	20.80	1.33	2.31
sidechain	21.93	1.97	3.01
waters	22.31		

$$* \quad R_{\text{sym}} = \frac{\sum |I_{\text{obs}} - I_{\text{avg}}|}{\sum I_{\text{avg}}}$$

† Numbers in parentheses represents the statistics for the shell comprising the outer 10% (theoretical) of the data.

‡ The percentage of scattering of the initial search model.

# Correlation obtained upon rigid-body refinement of the model against 8-4 Å data.

‡ Correlation in the D1 region of CD4 between the experimental electron density and the calculated model density (from CD4 as positioned by molecular replacement) using 10-2.8 Å data. Correlations in this region (consisting of ~6000 Å<sup>3</sup>) were used to generate a quantitative measure of the overall quality of

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the ternary complex experimental electron density. For the purposes of these calculations, the model used for phase combination omitted D1. A correlation of 0.6 is roughly the level of an interpretable protein electron density map, while a well refined structure would give a correlation of about 0.9.

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#### Fourth Series of Experiments

Human immunodeficiency virus (HIV-1) establishes persistent infections in humans leading to the acquired immune deficiency syndrome (AIDS). The HIV-1 envelope glycoproteins, gp120 and gp41, are assembled into a trimeric complex that mediates virus entry into target cells (1). HIV-1 entry depends upon the sequential interaction of the gp120 exterior envelope glycoprotein with the receptors on the cell, CD4 and members of the chemokine receptor family (2-4). The gp120 glycoprotein, which can be shed from the envelope complex, elicits both virus-neutralizing and non-neutralizing antibodies during natural infection. Antibodies that lack neutralizing activity are often directed against the gp120 regions occluded on the assembled trimer and exposed only upon shedding (5,6). Neutralizing antibodies, by contrast, must access the functional envelope glycoprotein complex (7) and typically recognize conserved or variable epitopes near the receptor-binding regions (8-11). Here, we describe the spatial organization of conserved neutralization epitopes on gp120, utilizing epitope maps in conjunction with the X-ray crystal structure of a ternary complex that includes a gp120 core, CD4 and a neutralizing antibody (12). A large fraction of the predicted accessible surface of gp120 in the trimer is composed of variable, heavily glycosylated core and loop structures that surround the receptor-binding regions. Understanding the structural basis for the ability of HIV-1 to evade the humoral immune response should assist vaccine design.

In primary sequence, human and simian immunodeficiency virus gp120 glycoproteins consist of five variable regions (V1-V5) interposed among more conserved regions (13). Variable regions V1-V4 form exposed loops

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anchored at their bases by disulfide bonds (14).

Neutralizing antibodies recognize both variable and conserved gp120 structures. The V2 and V3 loops contain  
5 epitopes for strain-restricted neutralizing antibodies (15-17). More broadly neutralizing antibodies recognize discontinuous, conserved epitopes in three regions of the gp120 glycoprotein (Table 1). In HIV-1 infected  
10 humans, the most abundant of these are directed against the CD4 binding site (CD4BS) and block gp120-CD4 interaction (8,9). Less common are antibodies against epitopes induced or exposed upon CD4 binding (CD4i) (18). Both CD4i and V3 antibodies disrupt the binding of gp120-CD4 complexes to chemokine receptors (10, 11).  
15 A third gp120 neutralization epitope is defined by a unique monoclonal antibody, 2G12, (19) which does not efficiently block receptor binding (11).

In an accompanying article, (12) we report the X-ray  
20 crystal structure of an HIV-1 gp120 core in a ternary complex with two-domain soluble CD4 and the Fab fragment of the CD4i antibody, 17b. The gp120 core lacks the V1/V2 and V3 variable loops, as well as N- and C-terminal sequences, which interact with the gp41  
25 glycoprotein, (6) and is enzymatically deglycosylated (12,21). Despite these modifications, the gp120 core binds CD4 and antibodies against CD4BS and CD4i epitopes (21, 22) and thus retains structural integrity. The gp120 core is composed of an inner domain, an outer  
30 domain and a third element, the "bridging sheet" (12) (Figure 34a). All three structural elements contribute, either directly or indirectly, to CD4 and chemokine receptor binding (12). Here, the organization of the surface of the gp120 is analyzed in light of the known  
35 antibody responses directed against this exposed viral glycoprotein.

### Variability and glycosylation of the gp120 surface

Although generally well-conserved compared with the five variable regions, some variability in the surface of the gp120 core is evident when the sequences of all primate immunodeficiency viruses are analyzed. This variability is disproportionately associated with the surface of the outer domain proximal to the V4 and V5 regions and removed from the receptor-binding regions (Figure 34a,b,c). The  $L_A$ ,  $L_C$ , and  $L_E$  surface loops (12) contribute to the variability of this surface. The potential N-linked glycosylation sites present in the gp120 core are concentrated in this variable half of the protein (Figure 34, b and c). In fact, the only conserved residues apparent on this relatively variable surface are asparagine 356 and threonine/serine 358, which constitute a complex carbohydrate addition site within the  $L_E$  loop (Figure 34, b and c). Since most carbohydrate moieties may appear as "self" to the immune system, the extensive glycosylation of the outer domain surface may render it less visible to immune surveillance. This helps to explain why antibodies directed against this gp120 surface have been identified so infrequently.

The receptor-binding regions retained in the gp120 core are well-conserved among primate immunodeficiency viruses (12). Also highly conserved is the surface of the inner domain spanned by the  $\alpha 1$  helix and located opposite the variable surface described above (Figure 34d). This surface is likely to interact with gp41 and/or with N-terminal gp120 segments absent from the gp120 core. This inner domain surface and the receptor-binding regions are devoid of glycosylation.

### Conserved gp120 neutralization epitopes

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In conjunction with prior mutagenic and antibody competition analyses (5,6, 18-21), the gp120 core structure reveals for the first time the spatial positioning of the conserved gp120 neutralization epitopes. Although the major variable loops are either absent (V1/V2 and V3) or poorly resolved (V4) in the gp120 core structure, their approximate positions can be deduced (Figure 35a). The conserved gp120 neutralization epitopes are discussed in relation to these variable loops and to the variable, glycosylated core surface.

a) CD4i epitopes. The gp120 epitope recognized by the CD4i antibody, 17b, can be directly visualized in the crystallized ternary complex (12) (Figure 35b,c). Strands from the gp120 fourth conserved (C4) region and the V1/V2 stem contribute to an antiparallel  $\beta$ -sheet (the "bridging sheet" (see Figure 34a)) that contacts the antibody. The vast majority of gp120 residues previously implicated in formation of the CD4i epitopes (18) (Table 1) are located either within this  $\beta$ -sheet or in nearby structures. With the exception of Thr 202 and Met 434, the gp120 residues in contact with the 17b Fab are highly conserved among HIV-1 isolates (Figure 34c, 2a). The prominent ("male") CDR3 loop of the 17b heavy chain dominates the contacts with gp120, with additional contacts through the heavy chain CDR2 (12).

Unusually, there are minimal 17b light chain contacts, leaving a large gap between the gp120 core and most of the 17b light chain surface. In the complete gp120 glycoprotein, this gap is likely occupied by the V3 loop. This is consistent with the position and orientation of the V3 stem on the gp120 core structure

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(12), the effect of V3 deletions on the binding of CD4i antibodies in the absence of soluble CD4 (22), the competition of some V3-directed antibodies with CD4i antibodies (5), and the ability of both antibody groups to block chemokine receptor binding (10,11). The chemokine receptor-binding region of gp120 likely consists of elements near or within the "bridging sheet" and the V3 loop (Figure 34a), a model that is supported by recent mutagenic analysis (C. Rizzuto and J. Sodroski, submitted).

The V2 loop likely resides on the side of the 17b epitope opposite the V3 loop (Figure 35a). The V1/V2 loops, which vary from 57 to 86 residues in length (13), are dispensable for HIV-1 replication (22,27), but decrease the sensitivity of viruses to neutralization by antibodies against V3 and CD4i epitopes (27). The latter effect is mediated primarily by the V2 loop (22), suggesting that part of the V2 loop folds back along the V1/V2 stem to mask the "bridging sheet" and adjacent V3 loop. The proximity of the V2 and V3 loops is supported by the observation that, in monkeys infected with simian-human immunodeficiency viruses (SHIVs), neutralizing antibodies are raised against discontinuous epitopes with V2 and V3 components (B. Etemad-Moghadam and J. Sodroski, submitted). The CD4i epitopes are probably masked by the flanking V2 and V3 loops, requiring the evolution of antibodies with protruding ("male") CDRs to access these conserved epitopes. CD4 binding has been suggested to reposition the V1/V2 loops, thus exposing the CD4i epitopes (22). The presence of contacts between the V1/V2 stem and CD4 in the crystal structure (12) is consistent with this model.

b) CD4BS epitopes. CD4 makes a number of contacts within a recessed pocket on the gp120



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surface. The gp120-CD4 interface includes two cavities, one water-filled and bounded equally by both proteins, the other extending into the gp120 interior and contacting CD4 only at phenylalanine 43 (Figure 34a (12). Table 1 and Figure 35b,c show the gp120 residues implicated in the formation of CD4BS epitopes recognized by eight representative antibodies. CD4BS epitopes are uniformly disrupted by changes in Asp 368 and Glu 370 (20), which surround the opening of the "Phe 43 cavity." These residues are located on a ridge at the intersection of the two receptor-binding gp120 surfaces, consistent with competition studies suggesting that CD4BS epitopes overlap both the CD4i epitopes and the binding site for CD4 (5,18). The location of the gp120 residues implicated in the formation of the CD4BS epitopes suggests that important elements of the CD4-binding surface of gp120 are accessible to antibodies.

Some CD4BS antibodies, like IgG1b12, are particularly potent at neutralizing HIV-1 (23). IgG1b12 binding is disrupted by gp120 changes that affect the binding of other CD4BS antibodies but, atypically, is sensitive to changes in the V1/V2 stem-loop structure (24). The observation that some well-conserved residues in the gp120 V1/V2 stem contact CD4 (12) raises the possibility that this protruding structure also contributes to the IgG1b12 epitope. This might increase the ability of the antibody to access the assembled envelope glycoprotein trimer, thus increasing neutralizing capability.

While the CD4BS epitopes and the CD4-binding site overlap, several observations demonstrate that the binding of CD4BS antibodies differs from that of CD4.

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Changes in Trp 427, a gp120 residue that contacts both the "Phe 43 cavity" and CD4, uniformly disrupt CD4 binding but affect the binding of only some CD4BS antibodies (Table 1). Conversely, some changes in other cavity-lining gp120 residues, Ser 256 and Thr 257, affect the binding of CD4BS antibodies more than the binding of CD4 (20). Since the recessed position of Ser 256 and Thr 257 in the current crystal structure (Figure 35b,c) makes direct contacts with antibody unlikely, either the effects of changes in these residues are indirect or the CD4BS antibodies recognize a gp120 conformation that differs from the CD4-bound state. With respect to the latter possibility, it is interesting that several of the residues implicated in the integrity of the CD4BS epitopes are located in the interface between the inner and outer gp120 domains. CD4BS antibodies might recognize a gp120 conformation in which the spatial relationship between the domains is altered compared with the CD4-bound state, thus allowing better surface exposure of these residues. Differences between the CD4BS epitopes and the CD4-binding site create opportunities for neutralization escape (20). The gp120 residues surrounding the "Phe 43" cavity are highly conserved among primate immunodeficiency viruses (Figure 35a), but the observed modest variation in adjacent surface-accessible residues (e.g., Pro 369, Thr 373 and Lys 432) could account for decrease recognition of the gp120 glycoprotein from some geographic clades of HIV-1 by CD4BS antibodies (24). Additional potential for variation near or within the CD4BS epitopes is created by the unusual water-filled cavity in the gp120-CD4 binding interface, since CD4 binding can apparently tolerate change in the gp120 residues contacting this cavity (12).

The recessed nature of the CD4 binding pocket on gp120 (Figure 34c) may delay the generation of high-affinity

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antibodies against the CD4BS epitopes and may afford opportunities to minimize the antiviral efficacy of such antibodies once they are elicited. The degree of recession is probably much greater on the full-length, glycosylated gp120 than is evident on the crystallized gp120 core. The recessed pocket is flanked on one side by the V1/V2 stem-loop structure. The characterization of HIV-1 escape mutants from the IgG1b12 CD4BS antibody and the mapping of several V2 conformational epitopes support a model in which the V2 loop folds back along the V1/V2 stem, with V2 residues 183-188 proximal to Asp 368 and Glu 370. This model is consistent with observations that V1/V2 changes, in combination with V3 changes, can alter the exposure of the adjacent CD4BS epitopes, particularly on the assembled trimer (28). The high temperature factors associated with the V1/V2 stem (12) imply flexibility in this protruding element (Figure 34c,d), expanding the potential range of space occupied by the V1/V2 stem-loop structure. This could enhance masking of the adjacent CD4BS and CD4i gp120 epitopes and divert antibody responses towards the variable loops.

Glycosylation may modify the interaction of antibodies with CD4BS epitopes. The L<sub>5</sub> loop, on the rim of the CD4-binding pocket opposite the V1/V2 stem, contains a well-conserved glycosylation site, asparagine 276 (Figure 34c). Changes in this site and at the adjacent alanine 281 have been associated with escape from the neutralizing activity of patient sera (25) and have been seen in SHIVs extensively passaged in monkeys (26). Another conserved glycosylation site at asparagine 386 lies adjacent to both CD4BS and CD4i epitopes (Figure 34c) and could diminish antibody responses against those sites. Additionally, in various HIV-1 strains, carbohydrates are added to the V2 loop segment (residues 186-188) thought to be proximal to the CD4BS epitopes.

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c) The 2G12 epitope. The integrity of the 2G12 epitope is disrupted by changes in gp120 glycosylation, either by glycosidase treatment or mutagenic alteration of specific N-linked carbohydrate addition sites (19). These sites are located on the relatively variable surface of the gp120 outer domain, opposite to and approximately 25 Å away from the CD4 binding site (Figure 35b,c). The gp120 glycoprotein synthesized in mammalian cells exhibits a dense concentration of high-mannose sugars in this region (Figure 35a). Even in the enzymatically deglycosylated gp120 core, carbohydrate residues constitute much of this surface. 2G12 likely binds at least in part to these carbohydrates, explaining the surprising conservation of the 2G12 epitope despite the variability of the underlying protein surface, which includes the stem of the V3 loop and the V4 variable region. The inclusion of carbohydrate in the epitope might also explain the apparent rarity with which these antibodies are generated. The localization of the 2G12 epitope is consistent with previous studies indicating that 2G12 forms a unique competition group (5,19) and does not interfere with the binding of monomeric gp120 to either CD4 or chemokine receptors (11). Since the 2G12 epitope is predicted to be oriented towards the target cell upon CD4 binding (see below), the antibody may sterically impair interactions of the oligomeric envelope glycoprotein complex with host cell moieties.

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Orientation of gp120 in the trimer

Possible orientations of the exterior glycoproteins in the trimer are significantly constrained by the requirement that observed and deduced binding sites for receptors and neutralizing antibodies, sites of N-linked glycosylation, and variable structures be exposed on the surface of the assembled complex. The two-domain CD4 in the ternary complex structure was aligned to the structure of four-domain CD4 (29) to orient the trimer model with respect to the target cell membrane. The consequences of such a model (Figure 36) are:

- a) the chemokine receptor-binding sites are clustered at the vertex of the trimer predicted to be closest to the target cell;
- b) both variable and conserved neutralization epitopes are concentrated on the half of gp120 facing the target cell;
- c) possibilities for intersubunit interactions among the variable structures that could help mask conserved neutralization epitopes are created;
- d) the subset of gp120 glycosylation sites to which complex carbohydrates are added in mammalian cells (14) is well-exposed on the outer periphery of the trimer;
- e) the highly conserved surface near the  $\alpha 1$  helix is available for gp41 and/or gp120 protein interactions within the trimers; and
- f) the surface of the assembled envelope glycoprotein complex is roughly hemispherical, thus minimizing the surface area of the viral spike that is potentially exposed to antibodies.

In summary, the X-ray crystal structure of the gp120 core/two-domain CD4/17b Fab complex provides a framework

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for visualizing key interactions between HIV-1 and the humoral immune system. Previous antibody competition analyses suggested that the gp120 surface buried in the assembled trimer elicits non-neutralizing antibodies (5,6). By contrast, the binding sites for neutralizing antibodies cluster on a different gp120 surface (5). Our structural studies support the existence of non-neutralizing and neutralizing faces of gp120, and reveal another, immunologically "silent" face of the glycoprotein (Figure 35d). This outer domain surface, along with the major variable loops, contributes to the large fraction of the gp120 surface that is protected against antibody responses by a dense array of carbohydrates and by the capacity for variation. The conserved receptor-binding regions of gp120 represent attractive targets for immune intervention. However, the elicitation of antibodies against these conformation-dependent structures is inefficient. Since the gp120 epitopes near the receptor-binding regions span the inner and outer domains, interdomain conformational shifts may decrease their representation in the immunogen pool. The recessed nature of the CD4-binding site likely contributes to its poor immunogenicity. The sequential recognition of two receptors by primate immunodeficiency viruses allows the conserved elements of the chemokine receptor-binding site to be created or exposed only after CD4 binding has occurred. At that point, it is likely that the proximity of the chemokine-receptor binding site to the cell membrane sterically limits antibody binding. The evolution of primate immunodeficiency viruses that successfully persist despite the host immune response presents challenges to vaccine development. An understanding of the structures of the relevant gp120 epitopes should assist efforts to overcome these hurdles.

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### Material and Methods

Graphics. Molecular graphics were produced using Midas-Plus (University of California, San Francisco) and GRASP (30).

Assignment of variability. Variability in gp120 residues was assessed using an alignment of sequences derived from approximately 400 HIV-1, HIV-2 and simian immunodeficiency viruses (13). Residues were assigned variability indices and color coded as follows:

- Red : conserved in all primate immunodeficiency viruses;
- Orange: conserved in all HIV-1, including groups M and O and chimpanzee isolates;
- Yellow: some variation among HIV-1 isolates (divergence from the consensus sequence in 1-8 of the 12 HIV-1 groups examined);
- Green : variable among HIV-1 isolates (divergence from the consensus sequence in  $\geq 9$  of the 12 HIV-1 groups examined).

Molecular modeling. Residues 88, 89, and 397-409, which are disordered in the ternary complex crystals (12), were built manually using the program TOM. For the V4 loop (residues 397-409), a dominant constraint was the distance between the ordered residues 396 and 410 ( $C\alpha$  -  $C\alpha$  distance of 26.88 Å). For the carbohydrate, examination of the N-linked carbohydrate in several crystal structures (e.g. 1fc2, 1gly, 1lte) showed that the core common to both high-mannose and complex N-linked sugars, (NAG)<sub>2</sub>(MAN)<sub>3</sub>, did not differ greatly in conformation after alignment of the first NAG. This core, which represents roughly half the total glycosylation for a typical N-linked site, was built onto each of the 18 consensus N-linked glycosylation sites found on the HXBc2 gp120 core. The

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stereochemistry of this initial model was refined using simulated annealing in XPLOR. Briefly, the model was heated to between 2,500° and 3,500°K, and "slow cooled" in steps of 25° to 300°K. At each step, molecular dynamics were performed with the core gp120 fixed, allowing only the modeled residues and carbohydrate (including any attached Asn) to move. The three separate runs, performing molecular dynamics for 5 fs/step, all steric clashes could be removed and the geometry idealized, with an average root mean square (RMS) of carbohydrate movement of only ~3.5Å. Four subsequent runs were made using dynamic times of between 50-75 fs/step. The carbohydrate positions obtained from these runs differed more substantially from those in the starting model (average carbohydrate RMS difference of roughly 8 Å). Two of the models from these longer annealings were much more similar to each other than to the rest (RMS differences in carbohydrate of ~ 4 Å versus ~ 8 Å for all other models). One had been heated to 3,500°K with dynamics of 75 fs/step. The other (shown in the figures display here) was heated to only 2,500°K with dynamics of 50 fs/step. In general the RMS movement of the NAG sugars was roughly half the RMS movement of the MAN sugars, reflecting greater conformational flexibility further from the protein surface.



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**Table 1. Conserved Epitopes for Neutralizing Antibodies Identified on the gp120 Core**

Competitive Group <sup>a</sup>	Examples of Monoclonal Antibodies	gp120 Amino Acids <sup>b</sup>	Probable Mechanism of Virus Neutralization	Characteristics	Selected References
C D 4 - Binding Site (CD4BS)	F105 15e 21h 1125h 448D 39.3 IgG1b12 830D	Asn 88 (13), Asp 113 (50), Lys 117 (25), Ser 256 (75), Thr 257 (75), Asn 262 (63), Ala 266 (13), Asp 368 (100), Glu 370 (100), Tyr 384 (13), Lys 421 (50), Trp 427 (25), Asp 457 (13), Pro 470 (25), Asp 474 (13), Met 475 (13), Asp 477 (63), Asp/Leu/Tyr 482/483/484 (25)	Interference with gp120-CD4 binding	C D 4 B S antibodies compete with CD4 and with antibodies against CD4i epitopes	8, 9, 20

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C D 4 - Induced Epitopes (CD4i)	17b 48d	Asn 88, Lys 117, Lys 121, Lys 207, Ser 256, Thr 257, Asn 262, ΔV3, Glu 370, Glu 381, Phe 382, Arg 419, Ile 420, Lys 421, Gln 422, Ile 423, Trp 427, Tyr 435, Pro 438, Met 475	Inter- ference with chemokine receptor binding	CD4 binding increases exposure of the epitopes as a result of movement of the V2 variable loop	18 and C. Rizzuto and J. Sodroski, submitted
2G12	2G12	Asn 295, Thr 297, Ser 334, Asn 386, Asn 392, Asn 397	Unknown	Antibody binding is dependent upon proper N- l i n k e d glycosylation	19

- <sup>a</sup> The gp120 competition groups are defined as Reference 5.
- <sup>b</sup> The gp120 amino acids are numbered according to the sequence of the HXBc2 (IIIB) gp120 glycoprotein, where residue 1 is the methionine at the amino-terminus of the signal peptide. Changes in the amino acids listed resulted in significant reduction in antibody binding to the gp120 glycoprotein (Ref. 18-20). The numbers in parentheses indicate the percentage of the CD4BC antibodies examined whose binding is decreased by changes in the indicated residue.

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Fifth Series of Experiments

The entry of primate immunodeficiency viruses into target cells depends upon a sequential interaction of the gp120 envelope glycoprotein with the cellular receptors, CD4 and members of the chemokine receptor family. The gp120 third variable (V3) loop has been implicated in chemokine receptor binding, but the use of the CCR5 chemokine receptor by diverse primate immunodeficiency viruses suggests the involvement of an additional, conserved gp120 element. Here we identify a highly conserved gp120 structure that is critical for CCR5 binding, is located adjacent to the V3 loop, and contains neutralization epitopes induced by CD4 binding. This conserved element may be a useful target for pharmacologic or prophylactic intervention in immunodeficiency virus infections.

The clinically abundant primate immunodeficiency viruses behind the  $\beta$ -chemokine receptor CCR5 as an obligate step in virus entry into target cells (1,2). The gp120 glycoproteins of primary, macrophage-tropic HIV-1 strains have been shown to bind specifically to cells expressing CCR5(3,4). The affinity of gp120 binding was increased 2-3 logs by the presence of soluble CD4 (sCD4) (3). Efficient CCR5 binding was dependent upon the presence of the V3 variable loop of gp120, but the gp120 V1/V2 variable loops and N- and C- termini were dispensable for high-affinity binding to CCR5(3). No significant CCR5 binding was observed for gp120 glycoproteins derived from laboratory-adapted HIV-1 isolates, which do not use CCR5 as a coreceptor (3,4).

Specific groups of HIV-1 neutralizing antibodies directed against the gp120 V3 loop or CD4-induced (CD4i) epitopes were able to block the binding of gp120-sCD4 complexes to CCR5-expressing cells (3,4). The CD4i

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epitopes are conserved, discontinuous gp120 structures that are exposed better after CD4 binding (5). Mutagenic analysis suggested that elements of the conserved stem of the V1/V2 stem-loop and of the fourth conserved region of gp120 comprise the CD4i epitopes (5). Here we test the hypothesis that conserved gp120 residues near or within the CD4i epitopes are critical for CCR5 binding.

10 An assay was established that could assess the CCR5-binding ability of a panel of HIV-1 gp120 glycoproteins mutants. The mutants were created by the introduction of single amino acid changes in gp120 residues near or within regions previously shown to be important for the integrity of the CD4i epitopes (5). During the course of this work, structural information on the gp120 epitope recognized by a CD4i-directed antibody, 17b, became available (6) (see below) and was used to guide the mutagenesis. The wtΔ glycoprotein, which lacks the V1/V2 variable loops and the N-terminus and is derived from the YU2 primary macropage-tropic HIV-1 isolate (7), was the starting point for the studies (Fig. 37). This protein was chosen because it had been shown to bind CD4 and CD5 with high affinity (3,8,9). Furthermore, the use of this protein minimized the opportunities for indirect effects of gp120 amino acid changes on CCR5 binding (e.g., by repositioning the V1/V2 loops, which can mask CD4i epitopes (9). Metabolically labeled wtΔ and mutant derivatives were produced in 293T cells and incubated with mouse L1.2 cells stably expressing human CCR5(3), in either the absence or presence of sCD4. The cells were washed and lysed, and bound gp120 protein was detected by precipitation with a mixture of sera from HIV-1 infected individuals (10).

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The wtΔ protein efficiently bound to the L1.2 CCR5 cells in the presence of sCD4 (Fig. 38,A and B). Binding was



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dramatically reduced when sCD4 was not present in the assay. The wtΔ protein binding to the L1.2-CCR5 cells was inhibited by preincubation of the wtΔ protein with the 17b antibody. Binding was also inhibited by incubation of the L1.2-CCR5 cells with the 2D7 antibody against CCR5 (11) or with the CCR5 ligand, MIP-1β(12). The C11 antibody, which is directed against a gp120 region dispensable for CCR5 binding (3), did not block the binding of the wtΔ protein to the L1.2-CCR5 cells (data not shown). The wtΔ protein did not bind appreciably to the parental L1.2 cells not expressing CCR5, even in the presence of sCD4. These results suggest that the wtΔ protein binds CCR5 in a specific, CD4-dependent manner.

The binding of the panel of gp120 mutants to the L1.2-CCR5 cells in the absence and presence of sCD4 was measured. The recognition of the mutant proteins by sCD4 and by monoclonal antibodies that recognize discontinuous gp120 epitopes (5,13) was assessed in parallel (10). Changes in several gp120 amino acids resulted in dramatic reductions in the ability of the protein to bind to L1.2-CCR5 cells in the presence of sCD4 (Table 1 and Fig. 38C). In some cases (257 T/D, 370 E/Q and 383 F/S), the attenuated CD4-binding ability of the mutant proteins could account for the observed reduction in binding to the L1.2-CCR5 cells. In most cases, however, the mutant proteins that were deficient in CCR5 binding still bound sCD4 and at least one of the monoclonal antibodies recognizing discontinuous gp120 epitopes. As expected, some of the introduced amino acid changes decreased recognition by the 17b antibody. Interestingly, two of the gp120 amino acid changes (437 P/A, 442 Q/L) resulted in an increase in CCR5 binding compared with the wtΔ protein, even though CD4 binding was not significantly increased. In the absence of sCD4, the 437 P/A and 442 Q/L envelope glycoprotein

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mutants bound to the L1.2-CCR5 cells slightly better than the other mutants and the wt $\Delta$  protein, which exhibited very low levels of binding (Fig. 38A and data not shown).

5  
Recently, the structure of an HIV-1 gp120 core crystallized in a ternary complex with two-domain CD4 and the 17b Fab has been solved (6). The gp120 core is composed of an inner domain, an outer domain, and a  
10 "bridging sheet" (Fig. 39A). The "bridging sheet" is a four-stranded, antiparallel  $\beta$ -sheet that includes the V1/V2 stem and strands ( $\beta$ 20 and  $\beta$ 21) derived from the fourth conserved gp120 region. CD4 contacts gp120 residues in the outer domain and the "bridging sheet"  
15 (6). The gp120 residues implicated by our study in CCR5 binding are located near or within the "bridging sheet" (Figure 39, A and B. The "bridging sheet" is predicted to face the target cell after the envelope glycoproteins bind CD4 (6). Even more than the CD4-binding site, the  
20 gp120 region implicated in CCR5 binding is highly conserved among primate immunodeficiency viruses; this is particularly apparent in comparison to the remainder of the gp120 surface thought to be exposed on the assembled envelope glycoprotein complex (Fig. 39C) (6).  
25 The CD4i epitope for the 17b antibody is located near or within the "bridging sheet" (6), consistent with the ability of the antibody to block CCR5 binding (3,4). All of the individual gp120 residues in which changes disrupted recognition by the 17b antibody (Fig. 39D) are  
30 located close to the gp120-17b interface in the crystallized complex (Table 1). The binding of another antibody, CG10, which disrupts gp120-CCR5 interaction (3) and competes with the 17b antibody for gp120 binding (14), is also affected by changes in amino acid residues  
35 within or near the "bridging sheet" (Fig. 39E). The position and orientation of the V3 base in the structure (6), in conjunction with a number of mutagenic and

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antibody competition studies (15), suggest that the gp120 V3 loop resides proximal to the region implicated in CCR5 binding (Fig. 39A). For example, the binding of both CG10 and CD4i antibodies to gp120 can be disrupted by some V3 changes (5,14). Furthermore, several V3-directed antibodies compete with CD4i antibodies for gp120 binding (15).

Our observations suggest that the CCR5-binding site is likely composed of conserved gp120 elements near or within the "bridging sheet" and V3 loop residues. The latter might include more conserved structures (e.g. the aromatic or hydrophobic residue at position 317, altered in this study) as well as more variable structures (16) that determine the specific chemokine receptor used. Some of the gp120 residues identified in this and previous studies (16) as determinants of chemokine receptor utilization could modulate the interaction of the V3 loop and elements near the "bridging sheet". For example, studies of HIV-1 revertants (15) suggested a functional interaction of gp120 residue 440, shown here to influence CCR5 binding, with the V3 loop.

A subset of the gp120 residues in or near the "bridging sheet" likely contacts CCR5 directly. Most of the gp120 residues implicated in CCR5 binding exhibit reasonable solvent accessibility in the free gp120 core (Table 1), consistent with this possibility. The gp120 surface implicated in CCR5 binding is highly basic (6), potentially favoring interactions with the acidic CCR5 amino terminus, which has been shown to be important for gp120 binding (17,18). Additionally, hydrophobic interactions, similar to those seen for gp120-17b binding (6), may also contribute to the gp120-CCR5 interaction.

The exposure and/or formation of the CCR5-binding site

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of HIV-1 gp120 glycoproteins is dependent upon interaction with CD4 (3,4). CD4 binding has been shown to reposition the V1/V2 variable loops and thus expose the CD4i epitopes (9), which overlap the CCR5-binding region (3,4). However, since a gp120 glycoprotein lacking the V1 and V2 variable loops also exhibits CD4-dependent CCR5 binding (3), the interaction with CD4 must cause other conformational changes in gp120 related to the CCR5-binding site. Our results, which highlight the proximity of the two receptor-binding sites on gp120, provide likely explanations for the induction of such conformational changes. First, one of the components of the "bridging sheet", the V1/V2 stem, also contacts CD4(6). Thus, CD4 binding, which appears to distort the V1/V2 stem, may reposition this structure and allow the formation of the  $\beta$ -sheet important for CCR5 binding. In this respect, we note that a substitution of aspartic acid for threonine 123, which is located in the V1/V2 stem and contacts CD4, significantly decreases CCR5 binding. This substitution may disrupt CD4-induced conformational changes in the V1/V2 stem required for CCR5 binding. Second, the CD4-bound conformation of gp120 exhibits a cavity (the "Phe 43" cavity) within the gp120 interior(6). This cavity contacts the gp120 inner and outer domains as well as the "bridging sheet" and likely forms as a result of interdomain conformational changes in gp120 induced by CD4 binding(6). Since the "bridging sheet" lacks its own hydrophobic core and is thus dependent upon residues contributed by both inner and outer domains(6), any shift in orientation between these domains would alter the conformation of the "bridging sheet". Furthermore, CD4 binding could also alter the precise orientation of the "bridging sheet" with respect to the inner and outer domains, thus aligning the V3 loop and conserved gp120 elements important for CCR5 binding. To summarize, CD4 binding likely induces conformational changes within the

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"bridging sheet" as well as between this sheet and the inner and outer domains to form the high-affinity CCR5 binding site. For some primate immunodeficiency viruses, the CD4-bound conformation of gp120 must be energetically assessable in the absence of CD4 to explain the documented examples of CD4-independent chemokine receptor binding and entry (18,19).

It is likely that the CCR5-binding region defined in this study is also important for the binding of simian and human immunodeficiency viruses to other chemokine receptors. The identified region exhibits one of the most highly conserved surfaces on the HIV-1 gp120 glycoprotein (6), supporting its functional importance for all primate immunodeficiency viruses. The laboratory-adapted HXBc2 envelope glycoprotein, which uses CXCR4 and not CCR5 as a coreceptor (1,2,20), can be converted to an efficient CCR5-using protein simply by substituting the V3 loop of the YU2 virus (2). Thus, all of the CCR5-binding region outside of the V3 loop must be conserved, at least between the HXBc2 and YU2 viruses. Indeed, we have shown that alteration of the lysine 117, lysine 207 and glycine 441 in the HXBc2-YU2V3 chimeric protein also disrupts CCR5 binding (21). Consistent with the use of this region for the binding of other chemokine receptors is the observation (19) that the gp120 changes associated with the conversion of HIV-2 to a CD4-independent, CXCR4-using virus affect the "bridging sheet" and the V3 loop. Alterations in "bridging sheet" residues have also been implicated in changes in the tropism of HIV-1 for immortalized cell lines that do not express CCR5(22). Finally, the 17b antibody neutralizes HIV-1 strains that use different chemokine receptors (5, 14), supporting the involvement fo a common gp120 region in chemokine receptor interaction.

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Chemokine receptor binding may trigger additional conformatinal changes in the envelope glycoprotein complex that ultimately lead to the fusion of the viral and target cell membrane. It is believed that some of these changes include exposure of the ectodomain of the gp41 transmembrane envelope glycoprotein(23). It is interesting that the CCR5-binding region defined herein likely resides closes to the trimer axis of the assembled envelope glycoprotein complex(6). Indeed, some of the gp120 residue changes that affect CR5 binding also affect the non-covalent association of gp120 and gp41 subunits in the trimeric complex(21). These observations raise the possibility that chemokine receptor binding alters the relationship between gp120 and gp41, leading to the exposure of the gp41 ectodomain and interaction with the target cell membrane.

The definition of a highly conserved gp120 structure that this important for binding to CCR5, the major coreceptor used by clinically abundant primate immunologic inhibitors of virus-receptor interactions. An understanding of the CD4-induced conformational changes in this structure may allow the targeting of sucg inhibitors to native or CD4-bound states of gp120.

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10. 293T cells were cotransfected with 20  $\mu$ g of a plasmid expressing the wt $\Delta$  or mutant envelope glycoproteins and 2  $\mu$ g of a plasmid expressing the HIV-1 Tat protein, using the calcium phosphate technique. Transfected cells were washed and metabolically labeled for 16 hours with 50  $\mu$ Ci/ml  $^{35}$ S-cysteine and 50  $\mu$ Ci/ml (35)S-methionine. Labeled cell supernatants were harvested, cleared by low-speed centrifugation (200 xg for 10 minutes at 4°C) and stored at 4°C until used in the binding assays.

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For measurement of the binding of sCD4 and antibodies to the wtΔ and mutant envelope glycoproteins, different dilutions of the envelope glycoprotein-containing supernatants were precipitated to ensure that binding occurred in the linear range of the assay. For CD4 binding, the envelope glycoprotein-containing supernatants were incubated for 30 minutes at room temperature with a concentration of sCD4 (Smith Kline Beecham) empirically determined to precipitate the wtΔ protein optimally. The envelope glycoprotein-sCD4 complexes were then precipitated with the CD4-specific antibody, OKT4 (Ortho) and Protein A-Sepharose (Pharmacia). For binding of the 17b and F105 antibodies, the monoclonal antibodies were preincubated with Protein A-Sepharose prior to overnight incubation with envelope glycoprotein-containing supernatants at 4°C. For Binding of the CG10 antibody, envelope glycoprotein-containing supernatants were incubated with 100 nM sCD4 at room temperature for 30 minutes prior to addition of a CG10-Protein G-Sepharose mixture and overnight incubation at 4°C. Immunoprecipitates were washed and run on 12.5% SDS-polyacrylamide gels, which were fixed, dried and analyzed by autoradiography. Binding was qualified by densitometry.

To measure CCR5 binding, envelope glycoprotein-containing supernatants were mixed with 100nM xCD4 or phosphate-buffered saline (PBS) and incubated at room temperature for 30-60 minutes. L1.2-CCR5 cells ( $2 \times 10^7$  cells, LeukoSite, Inc.(3)) were pelleted, resuspended in 500  $\mu$ l of envelope glycoprotein-containing supernatants, and rocked gently at 37°C for 1 hour. Cells were pelleted, washed twice in PBS and lysed by the addition of NP40 buffer (0.5 M NaCl, 10 mM Tris, pH 7.5, 0.5%



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NP40). Lysates were cleared (20,000 xg at 4°C for 15 minutes) in a microcentrifuge and the envelope glycoproteins were precipitated overnight at 4°C by a mixture of sera from HIV-1-infected individuals and Protein A-Sepharose. Sepharose pellets were washed in NP40 buffer, boiled in SDS-containing sample buffer and run on 12.5% SDS-polyacrylamide gels. Autoradiographed gels were quantitated using a densitometer.

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10 Table 1. Phenotypes of HIV-1 gp120 mutants. The ability of the wtΔ and mutant glycoproteins to bind CCR5 expressed on L1.2 cells was determined (10). The recognition of the wtΔ and mutant glycoproteins by sCD4 and monoclonal antibodies was determined (10). All values reported are relative to those seen for the wtΔ

15 protein. Values represent the average of at least two independent experiments and exhibited less than 30% variation from the values shown.

Protein(Fractional Solvent Accessibility)*	Ligand Binding†				
	CCR5 Binding +	sCD4	17b	CG10	F105
wtΔ	1.00	1.00	1.00	1.00	1.00
107D/R	1.02	1.02	0.97	1.11	1.14
114Q/L	1.22	0.79	0.73	0.71	0.75
117 K/D (0.45)	0.15	0.74	0.64	0.42	0.83
121 K/D (0.57)	0.07	0.73	0.11	0.0	0.99
122 L/S	0.98	0.84	1.07	0.18	1.11
123 T/D (0.49)	0.08	0.99	1.06	0.0	1.25
197 N/D	1.33	1.34	.80	0.81	1.11
199 S/L	1.50	1.32	.94	1.03	1.04
200 V/S	0.84	0.91	1.05	0.49	1.06
201 I/A	0.46	0.90	.67	0.84	0.81
203 Q/L	0.68	0.85	.88	0.52	0.93
207 K/D (0.23)	0.0	0.85	.46	0.13	0.98

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209 S/L	1.00	1.11	.85	1.01	1.00
210 F/S	0.65	0.81	.81	0.85	0.74
211 E/K	0.73	1.13	1.03	1.12	1.24
257 T/D	0.05	0.0	.49	0.06	0.0
295 N/E	0.86	0.75	.73	0.98	0.79
308 N/D	0.31	1.10	.89	0.93	1.03
317 L/S	0.08	1.12	1.05	1.13	1.03
330 H/A	0.22	0.75	.55	0.66	0.64
$\Delta V3$ ( $\Delta 298-329$ )	0.0	0.80	0.08	1.27	0.93
370 E/Q	0.17	0.0	1.04	0.12	0.0
372 V/S	0.85	1.03	1.08	1.09	0.44
373 T/D	0.48	1.12	1.10	1.16	1.10
377 N/E (0.04)	0.22	0.71	0.52	0.65	0.60
381 E/R (0.07)	0.07	0.81	0.75	0.29	0.96
383 F/S	0.04	0.0	0.0	0.07	0.0
386 N/D	1.22	1.14	0.97	0.90	0.97
419 R/D (0.82)	0.19	0.86	0.02	0.48	0.82
420 I/R (0.14)	0.06	0.59	0.0	0.72	0.72
421 K/D (0.32)	0.07	0.86	0.19	0.0	0.0
422 Q/L (0.35)	0.07	0.53	0.0	0.20	0.55
423 I/S	0.61	0.97	0.05	0.30	1.03
424 I/S	0.37	0.25	0.48	0.83	0.81
426 M/A	0.75	0.69	0.69	0.72	1.11
429 E/R	1.54	1.17	1.00	1.05	0.82
432 K/A	0.61	1.0	0.92	0.0	1.45
434 M/A	1.22	.90	0.65	0.07	1.04
435 Y/S	0.21	.33	0.22	0.29	1.00
436 A/S	0.98	1.05	0.91	0.99	1.23
437 P/A	1.79	.80	0.68	0.78	0.82
438 P/A (0.28)	0.06	1.18	1.00	1.13	1.18
439 I/A	0.45	0.68	0.76	0.76	0.84
440 R/D (0.43)	0.09	1.03	1.05	1.05	1.13

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441 G/V (0.91)	0.0	.67	0.70	0.62	0.78
442 Q/L	2.00	1.11	0.74	1.05	0.83
444 R/D (0.80)	0.25	.79	0.67	0.94	0.74
474 D/R	1.03	.59	0.81	0.74	0.0

\*The number of the mutant wtΔglycoproteins is based on the sequence of the prototypic HXBc2 gp120 glycoprotein (24), with 1 representing the initiator methionine. The wild-type YU2 gp120 residue is listed, followed by the substituted residue. Amino acid abbreviations: A, Alanine; D, aspartic; E, glutamic acid; F, phenylalanine; G, glycine; h, histidine; I, isoleucine; K, lysine; L, leucine; M, methionine; N, Asparagine; P, proline; Q, glutamine; R, arginine; S, serine; T, threonine; V, valine; Y, tyrosine. The fractional solvent accessibilities associated with gp120 residues in which changes specifically disrupted CCR5 binding are shown in parentheses. Fractional solvent accessibility was calculated as the ratio of solvent-accessible surface area for atoms of amino-acid residue X in the gp120 core (without carbohydrate moieties) to the area obtained after reducing the structure to a Gl-X-Gly tripeptide (24), values cited are for side-chain atoms except for glycine 441 where the value for all atoms is given.

+The binding of the wtΔ glycoprotein to L1.2-CCR5 cells was shown to be linearly related to the concentration of wtΔ protein in the transfected 293T cell supernatants, over the range of concentrations used in these experiments. The total amount of wtΔ and mutant glycoprotein present in the 293T cell supernatants was estimated by precipitation with an excess of a mixture of sera from HIV-1-infected individuals. The amount of wtΔ and mutant glycoprotein bound to the L1.2-CCR5 cells was determined as described (10). The value for CCR5 binding was calculated using the following formula:

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Bound mutant protein      Total      wtΔ

protein

CCR binding=    Bound wtΔ protein    X    Total    mutant  
protein

5

‡The recognition of the wtΔ and mutant glycoproteins by  
sCD4 and antibodies was determined by precipitation of  
radiolabeled envelope glycoproteins in transfected 293T  
cell supernatants as described (10). In parallel, the  
labeled envelope glycoproteins were precipitated with an  
excess of a mixture of sera from HIV-1-infected  
individuals. The value for ligand binding was  
calculated using the following formula:

15    Ligand binding =  $\frac{\text{Mutant protein}_{\text{ligand}}}{\text{wtΔprotein}_{\text{ligand}}} \times \frac{\text{wtΔprotein}_{\text{serum mixture}}}{\text{Mutant protein}_{\text{serum mixture}}}$

In the sCD4 and 17b columns, the values in bold indicate  
gp120 residues that exhibit decreased solvent  
accessibility on the presence of the two-domain sCD4 or  
17b Fab, respectively, in the ternary complex (6).  
Changes in solvent accessibility were calculated using  
the MS program of Michael Connolly.

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What is claimed is:

1. A crystal suitable for X-ray diffraction comprising a polypeptide having an amino acid sequence of a portion of a Human Immunodeficiency Virus envelope glycoprotein gp120.  
5
2. The crystal of claim 1, which effectively diffracts X-rays for determination of the atomic coordinates of the polypeptide to a resolution of 4 angstroms or better than 4 angstroms.  
10
3. The crystal of claim 1, which effectively diffracts X-rays for determination of the atomic coordinates of the polypeptide to a resolution of 2.5 angstroms or better than 2.5 angstroms.  
15
4. The crystal of claim 1, wherein the portion of gp120 comprises a CD4 binding site.
- 20 5. The crystal of claim 4, further comprising a compound bound to the CD4 site.
6. The crystal of claim 1, wherein the portion of gp120 comprises a chemokine receptor binding site.  
25
7. The crystal of claim 6, further comprising a compound bound to the chemokine receptor binding site.
- 30 8. The crystal of claim 1, wherein the portion of gp120 comprises a CD4 binding site and a chemokine receptor binding site.
- 35 9. The crystal of claim 8, further comprising of a first compound bound to the CD4 binding site of the polypeptide and a second compound bound to the chemokine receptor binding site of the polypeptide.

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10. The crystal of claim 9, wherein the first compound is the second compound.
- 5 11. The crystal of claim 9, wherein the crystal is arranged in a space group  $P222_1$ , so as to form a unit cell of dimensions  $a=71.6 \text{ \AA}$ ,  $b=88.1 \text{ \AA}$ ,  $c=196.7 \text{ \AA}$ , and which effectively diffracts x-rays for determination of the atomic coordinates of the  
10 gp120 to a resolution of  $2.5 \text{ \AA}$  or better.
12. The crystal of claim 1, wherein the polypeptide is a variant of gp120 lacking the V1, V2, V3, and C5 regions.
- 15 13. The crystal of claim 12, wherein the gp120 variant comprises a portion of the conserved stem of the V1/V2 stem-loop structure.
- 20 14. The crystal of claim 13, wherein the gp120 variant comprises a portion of the base of the V3 loop.
15. The crystal of claim 14, wherein the gp120 variant comprises a portion of the C5 region.
- 25 16. The crystal of claim 1, wherein the polypeptide is a variant of gp120 with 5% by weight of the carbohydrate residues linked to the gp120 in substantially the same manner as they are linked to  
30 gp120 in unmodified gp120.
17. The crystal of claim 1, wherein the polypeptide is a variant of gp120 with 15% by weight of the carbohydrate residues linked to the gp120  
35 polypeptide in substantially the same manner as they are linked to gp120 in unmodified gp120.



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18. The crystal of claim 12 or 16, further comprising a Fab, a CD4, a polypeptide having amino acid sequence of a portion of CD4, or a combination thereof, bound to the gp120.
- 5
19. The crystal of claim 18, wherein the Fab is produced from an antibody to a discontinuous epitope.
- 10
20. The crystal of claim 19, wherein the monoclonal antibody is designated 17b.
21. A method for producing a crystal suitable for X-ray diffraction comprising:
- 15
- a. deglycosylating a polypeptide having amino acid sequence of a portion of a gp120 wherein said portion is produced by deleting or replacing part of the gp120 to reduce the surface loop flexibility;
- 20
- b. contacting the polypeptide with a ligand so as to form a complex which exhibits restricted conformational mobility; and
- c. obtaining crystal from the complex so formed to produce a crystal suitable for X-ray
- 25
- diffraction.
22. The method of claim 21, wherein the V1, V2, or V3 loop of the gp120 contained in the polypeptide are partially truncated, deleted or replaced.
- 30
23. The method of claim 21, wherein the polypeptide lacks the V1, V2, V3 and C5 loop of the gp120.
24. The method of claim 21, wherein the ligand is a
- 35
- Fab, a CD4, or a polypeptide having amino acid sequence of a portion of CD4.

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25. The method of claim 21, wherein the resulting polypeptide after the deglycosylation contains at least 5% of the carbohydrate.
- 5 26. The crystal produced by the method of claim 21.
27. A method for identifying a compound capable of binding to a portion of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising:
- 10 a. determining a binding site on the portion of gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising the portion of gp120; and
- 15 b. determining whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the gp120.
28. A method for designing a compound capable of binding to a portion of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising:
- 20 a. determining a binding site on the portion of gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising the portion of gp120; and
- 25 b. designing a compound to fit the binding site.
29. A method of claim 27 or 28, wherein the fitting is determined by shape complementarity or by estimated interaction energy.
- 30 30. A method of claim 27 or 28, wherein the atomic coordinates are set forth in Figure 53.
- 35 31. A pharmaceutical composition comprising the compound identified by claim 27 and a pharmaceutically acceptable carrier.

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32. The method of claim 27, wherein the compound is not previously known.
33. The compound identified by the method of claim 32.
- 5 34. The compound designed by the method of claim 28.
35. A composition comprising the compound of claim 34 and a suitable carrier.
- 10 36. A method of inhibiting the interaction of HIV-gp120 with CD4 which comprises administering to a mammal a compound, with the proviso that the compound is not CD4, capable of disrupting two or more of the contacts between gp120 and CD4 as set forth in Figure 54.
- 15 37. A method for identifying a compound capable of binding to the CD4 binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising:
- 20 a. determining the CD4 binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of gp120 capable of binding to CD4; and
- 25 and
- 30 b. determining whether a compound would fit into the binding site, a positive fitting indicating that the compound is capable of binding to the CD4 binding site of the gp120.
- 35 38. A method for designing a compound capable of binding to the CD4 binding site of Human Immunodeficiency Virus envelope glycoprotein gp120

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comprising:

- 5           a.    determining the CD4 binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide having amino acid sequence of a portion of gp120 capable of binding to CD4; and
- 10           b.    designing a compound to fit the CD4 binding site.
- 15           39.   A method of claim 37 or 38, wherein the crystal further comprising a CD4, a second polypeptide having amino acid sequence of a portion of CD4, or a compound known to be able to bind to the CD4 site of the gp120, bound to the polypeptide.
- 20           40.   A method of claim 37 or 38, wherein the fitting is determined by shape complementarity or by estimated interaction energy.
- 25           41.   A method of claim 37 or 38, wherein the atomic coordinates are set forth in Figure 53.
42.   A pharmaceutical composition comprising the compound identified by claim 37 and a pharmaceutically acceptable carrier.
- 30           43.   The method of claim 37, wherein the compound is not previously known.
44.   The compound identified by the method of claim 43.
- 35           45.   The compound designed by method of claim 38.
46.   A composition comprising the compound of claim 44

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or 45 and a suitable carrier.

47. A method of inhibiting Human Immunodeficiency Virus infection in a subject comprising administering effective of amount of the composition of claim 46 to the subject.
48. A method for identifying a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising:
- a. determining the chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide comprising the amino acid sequence of a portion of gp120 capable of binding to the chemokine receptor; and
  - b. determining whether a compound would fit into the binding site, a positive fit indicating that the compound is capable of binding to the chemokine receptor binding site of the gp120.
49. A method for designing a compound capable of binding to the chemokine receptor binding site of Human Immunodeficiency Virus envelope glycoprotein gp120 comprising:
- a. determining the chemokine receptor binding site on the gp120 based on the atomic coordinates computed from X-ray diffraction data of a crystal comprising a polypeptide comprising the amino acid sequence of a portion of gp120 capable of binding to the chemokine receptor; and
  - b. designing a compound to fit the chemokine receptor binding site.

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50. The method of claim 48 or 49, wherein the crystal further comprises a chemokine receptor, a second polypeptide having amino acid sequence of a portion of chemokine receptor, an antibody or a Fab capable of binding to the chemokine receptor binding site or a compound known to be capable of binding to the chemokine receptor binding site, bound to the polypeptide.
51. The method of claim 48 or 49, wherein the fitting is determined by shape complementarity or by estimated interaction energy.
52. The method of claim 48 or 49, wherein the atomic coordinates are set forth in Figure 53.
53. The pharmaceutical composition comprising the compound identified by the method of claim 48 and a pharmaceutically acceptable carrier.
54. The method of claim 48, wherein the compound is not previously known.
55. The compound identified by the method of claim 54.
56. The compound designed by method of claim 49.
57. A composition comprising the compound of claim 55 or 56 and a suitable carrier.
58. A method of inhibiting Human Immunodeficiency Virus infection in a subject comprising administering effective of amount of the composition of claim 57 to the subject, thereby inhibiting Human Immunodeficiency Virus infection.
59. A method of inhibiting the interaction of HIV-gp120

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with chemokine receptor which comprises administering to a mammal a compound capable of disrupting two or more of the contacts between gp120 and chemokine receptor as set forth in figure 55, thereby inhibiting the interaction of HIV-gp120 with chemokine receptor with the proviso that the compound is not a chemokine receptor.

60. The method of claim 59, wherein the compound is nonpeptidyl.

61. A substance mimicking the human immunodeficiency virus envelope glycoprotein gp120-binding region of CD4 wherein the size of a residue or analog thereof, corresponding to the phenylalanine at position 43 in the native CD4, is larger than the size of phenylalanine so as to fill the pocket on gp120 which extends beyond position 43 in the gp120/CD4 complex and increase the affinity for gp120.

62. The substance of claim 61, wherein the substance is a peptidomimetic analog, a synthetic polypeptide, a standard polypeptide, or a polypeptide analog.

63. The substance of claim 61, wherein the size of residue or analog thereof is increased by directly or indirectly linking a hydrophobic compound to the residue or analog thereof.

64. The substance of claim 61, wherein the sidechain of the residue or analog thereof is larger than 7 Å across its longest dimension.

65. The substance of claim 61, wherein the sidechain of the residue or analog is larger than 10 Å across its longest dimension.

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66. The substance of claim 61, wherein the sidechain of the residue or analog thereof is larger than 15 Å across its longest dimension.
- 5 67. The substance of claim 61, wherein the sidechain of the residue or analog thereof is longer than the phenylalanine sidechain's longest dimension.
- 10 68. The substance of claim 61, which enhances hydrophobic interactions to residues that line the pocket.
69. The substance of claim 61, which enhances hydrogen bonding to residues that line the pocket.
- 15 70. The substance of claim 61, which enhances electrostatic interactions with residues that line the pocket.
- 20 71. The substance of claim 61, which enhances surface fit with residues that line the pocket.
72. The substance of claim 61, wherein the residue or analog thereof contains a localization of charge so as to render the gp120-binding region of CD4 able to hydrogen bond more strongly with the hydroxyl-containing side chains lining gp120.
- 25 73. The substance of claim 61, wherein the residue or analog thereof contains at least one additional carbon group.
- 30 74. The substance of claim 61, wherein the modification involves replacement of the residue at position 43 with a cysteine and substitution of the sulfhydryl group.
- 35



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75. The substance of claim 61, wherein the modification involves replacement of the residue at position 43 with a tyrosine and substitution of the tyrosine.
- 5 76. The substance of claim 61, wherein the residue or analog thereof is directly or indirectly linked to an adaptor.
- 10 77. The substance of claim 76, wherein the adaptor residue or analog thereof is directly or indirectly linked to a hydrophobic compound to form a complex.
- 15 78. The substance of claim 77, wherein the formed complex is larger than 7 Å across its longest dimension.
79. The substance of claim 77, wherein the complex is larger than 10 Å across its longest dimension.
- 20 80. A pharmaceutical composition capable of inhibiting cell entry by human immunodeficiency virus, comprising
- a. an effective amount of the substance of claim 61; and
- 25 b. a pharmaceutically acceptable carrier.
81. A composition capable of inhibiting cell entry by human immunodeficiency virus, comprising
- a. an effective amount of a substance mimicking
- 30 the human immunodeficiency virus envelope glycoprotein gp120-binding region of CD4 wherein the size of a residue or analog thereof, corresponding to the phenylalanine at position 43 in the native CD4, is larger than
- 35 the size of phenylalanine so as to fill the pocket on gp120 which extends beyond position 43 in the gp120/CD4 complex and increase the

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affinity for gp120; and

b. a suitable carrier.

- 5 82. A pharmaceutical composition for treating or preventing human immunodeficiency virus infection, comprising
- a. an effective amount of the substance of claim 61; and
- 10 b. a pharmaceutically acceptable carrier.
83. A composition for treating or preventing human immunodeficiency virus infection, comprising
- a. an effective amount of the substance of claim 61; and
- 15 b. a suitable carrier.
84. A method of inhibiting cell entry by human immunodeficiency virus, comprising
- 20 contacting the cells with an effective amount of the substance of claim 61 to inhibit cell entry by human immunodeficiency virus.
85. A method of treating or preventing human immunodeficiency virus infection in a subject,
- 25 comprising administering to the subject an effective amount of the substance of claim 61, thereby treating or preventing human immunodeficiency virus infection.
- 30 86. A variant of gp120 which presents a hidden, conserved, neutralization epitope.
87. The variant of 86 wherein position 375 is changed from a Serine to a Trptophan.
- 35 88. The variant of claim 87 further comprising one of the following changes: 88N to P, 102E to L, 113D to

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R, 117K to W, 257T to A, 266A to E, 386N to Q, 395W to S, 421K to L, 470P to G, 475M to S, 485K to V or a combination thereof.

- 5      89. A composition comprising the variant of claim 86, 87 or 88 and a suitable carrier.
90. A vaccine comprising the variant of claim 86, 87 or 88.
- 10     91. A method for inducing antibody against HIV in a subject comprising administering an effective amount of the variant of claim 86 to the subject.
- 15     92. The method of claim 91, wherein the subject is a human.
93. The vaccine of claim 91, further comprising a suitable adjuvant.
- 20     94. An antibody against the variant of claim 86, 87 or 88.
95. The antibody of claim 94, wherein the antibody is neutralizing to HIV.
- 25     96. The antibody of claim 94, wherein the antibody is a monoclonal antibody.

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International Bureau



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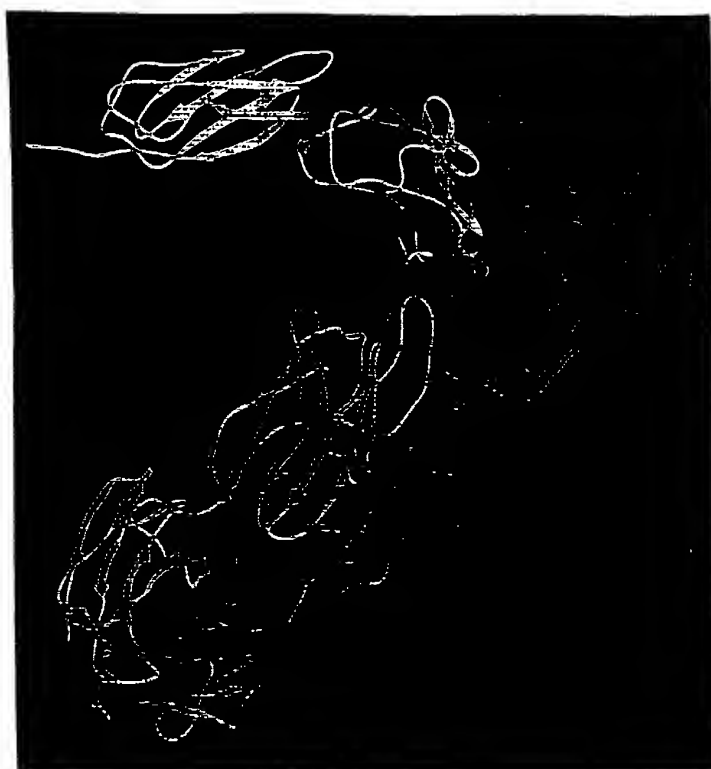
PCT

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CANCER INSTITUTE, INC. [US/US]; 44 Binney Street, Boston, MA 02115 (US).
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| 60/089,581 | 17 June 1998 (17.06.1998)     | US |
| 60/089,580 | 17 June 1998 (17.06.1998)     | US |
| 09/100,763 | 18 June 1998 (18.06.1998)     | US |
| 09/100,631 | 18 June 1998 (18.06.1998)     | US |
| 09/100,529 | 18 June 1998 (18.06.1998)     | US |
| 09/100,762 | 18 June 1998 (18.06.1998)     | US |
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- (71) Applicants (*for all designated States except US*): THE TRUSTEES OF COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK [US/US]; West 116th Street and Broadway, New York, NY 10027 (US). DANA-FARBER
- (54) Title: CRYSTAL COMPRISING HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN gp120, COMPOUNDS INHIBITING CD4-gp120 INTERACTION, COMPOUNDS INHIBITING CHEMOKINE RECEPTOR-gp120 INTERACTION, MIMICS OF CD4 AND gp120 VARIANTS
- (57) Abstract: The subject invention provides a crystal suitable for X-ray diffraction comprising a polypeptide having an amino acid sequence of a portion of a Human Immunodeficiency Virus envelope glycoprotein gp120. The subject invention also provides the above-described crystals, wherein the crystal is arranged in a space group P222<sub>1</sub>, so as to form a unit cell of dimensions a=71.6 Å, b=88.1 Å, c=196.7 Å, and which effectively diffracts X-rays for determination of the atomic coordinates of the gp120 to a resolution of 2.5 Å or better. The subject invention additionally provides compounds inhibiting the CD4-gp120 interaction, compounds inhibiting chemokine receptor-gp120 interaction, mimics of CD4, gp120 variants and uses thereof.

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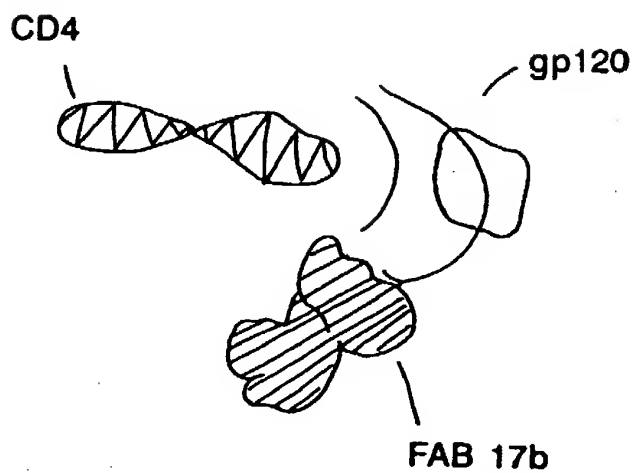
FIG. 1



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FIG. 2

gp120/17/CD4 Complex  
Structure



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FIG. 3B

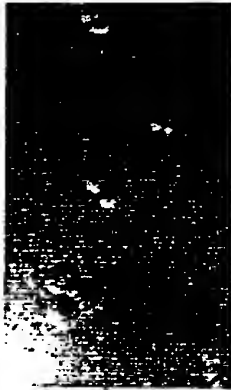


FIG. 3D



FIG. 3F

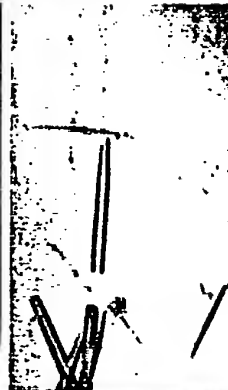


FIG. 3A



FIG. 3C



FIG. 3E



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FIG. 4





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FIG. 5A



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FIG. 5B



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FIG. 6



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FIG. 7



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FIG. 8



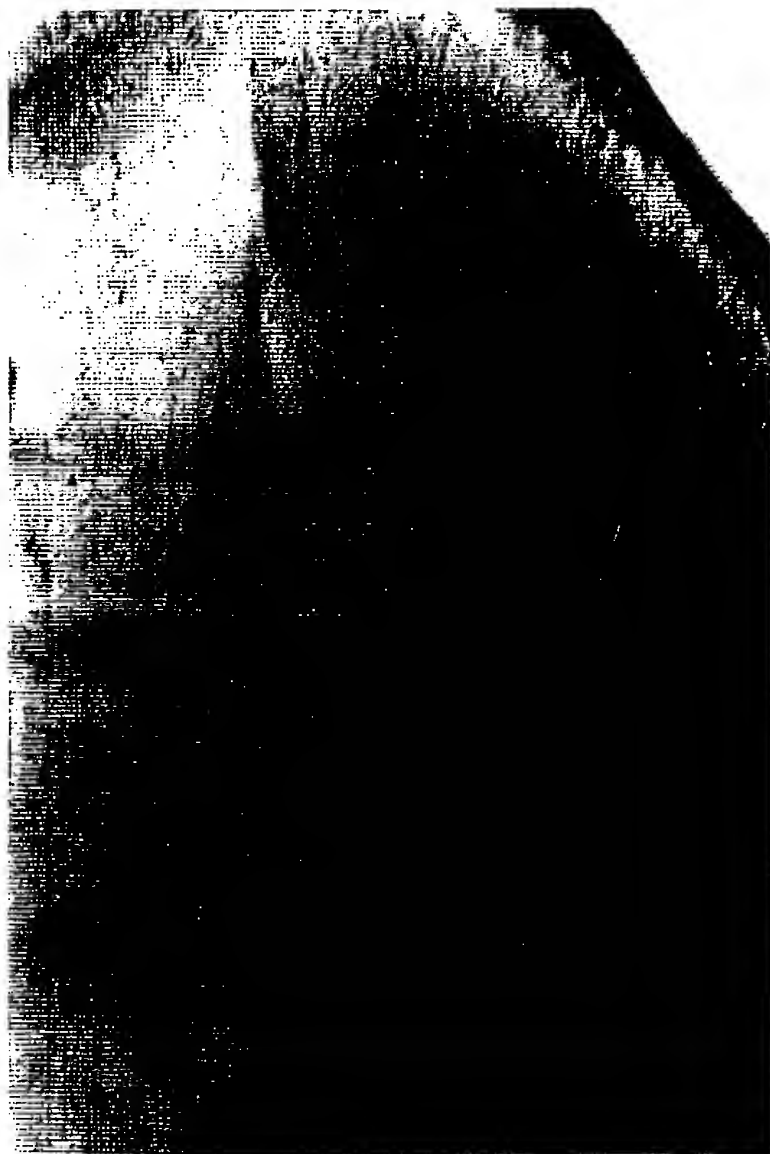
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FIG. 9



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FIG. 10



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FIG. 11





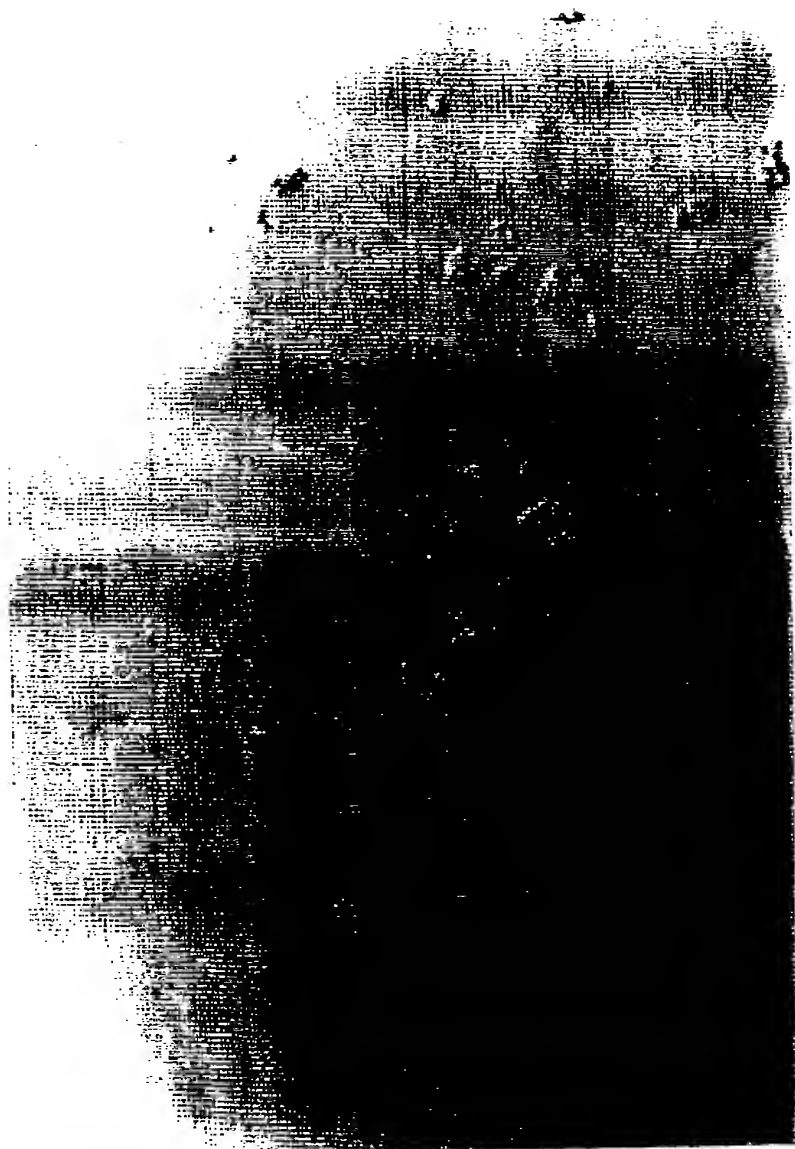
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FIG. 12



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FIG. 13



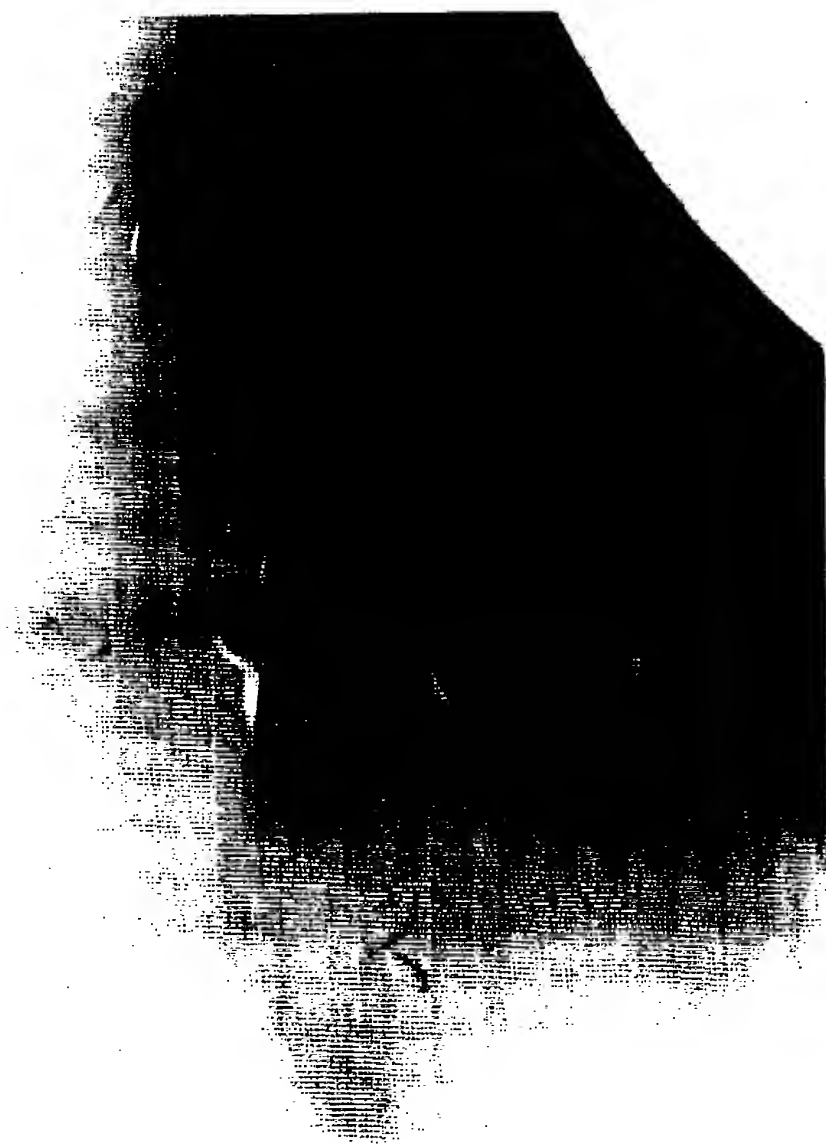
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FIG. 14



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FIG. 15



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FIG. 16



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FIG. 17



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FIG. 18



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FIG. 19





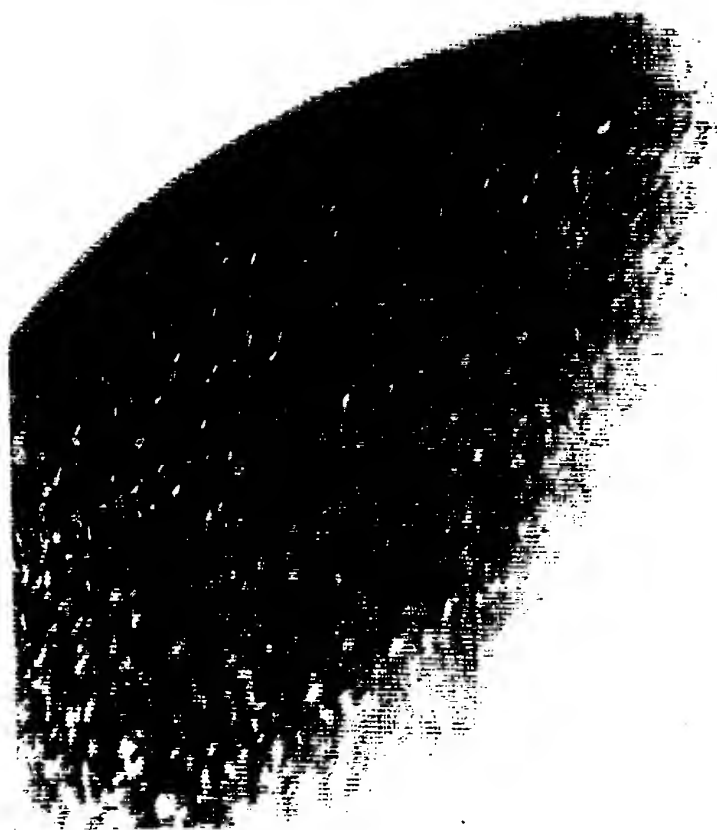
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FIG. 20



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FIG. 21



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FIG. 22



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FIG. 23



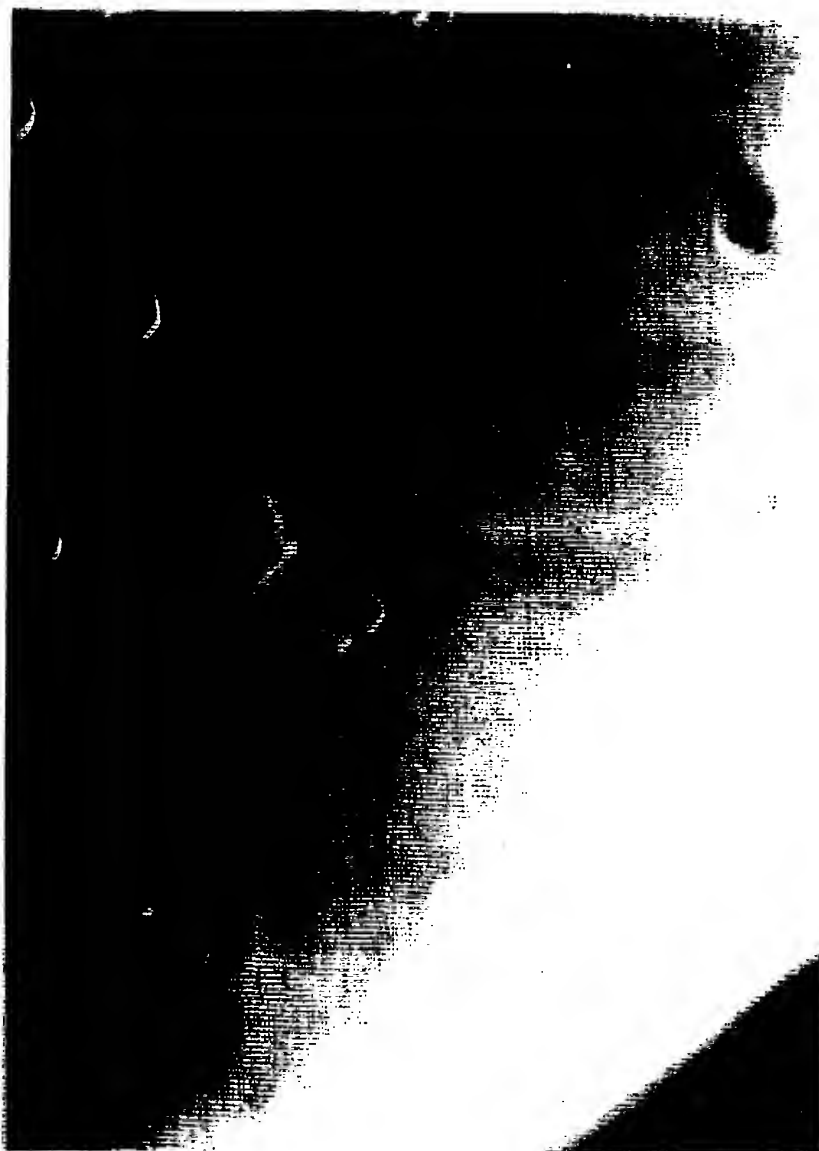
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FIG. 24



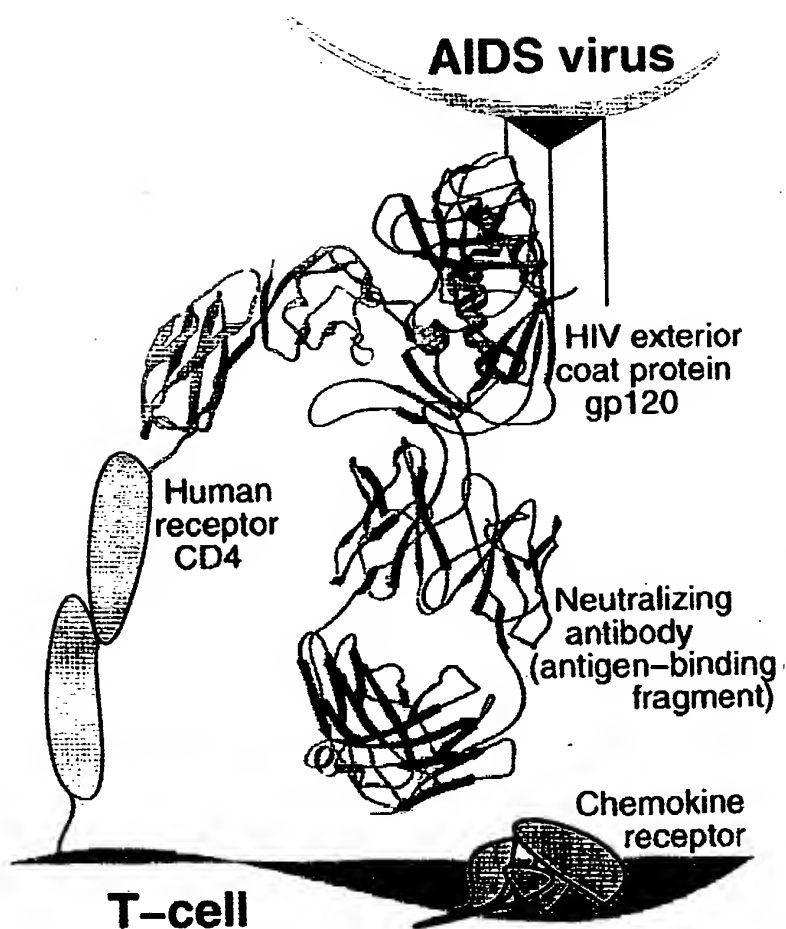
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FIG. 25



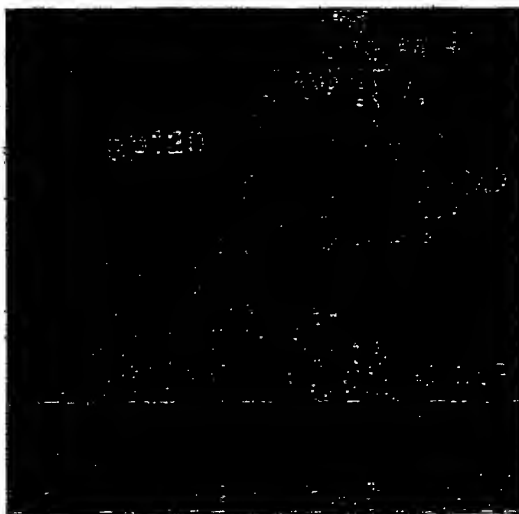
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FIG. 26A



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FIG. 26B





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FIG. 27A

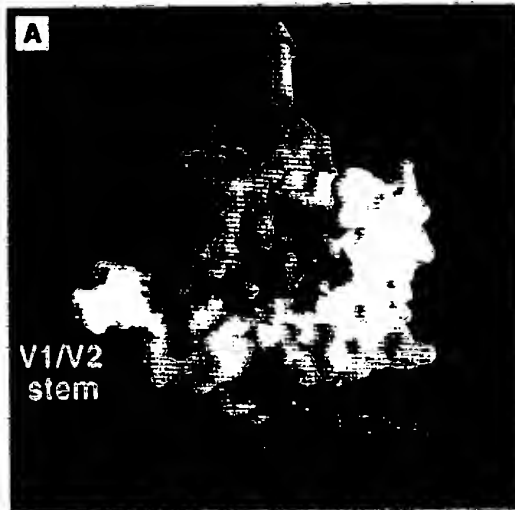


FIG. 27B

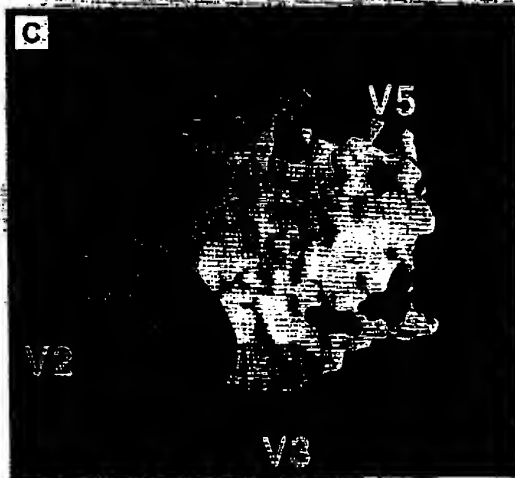
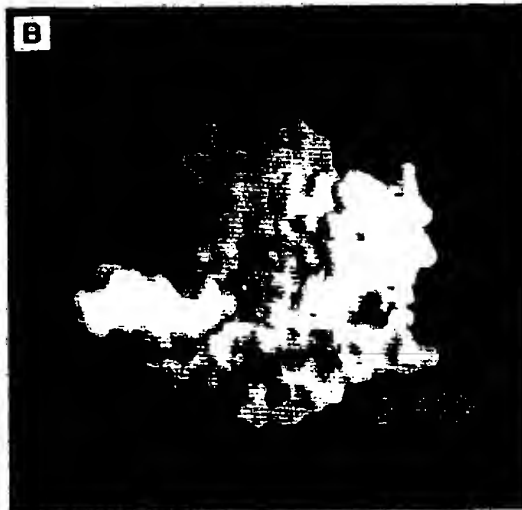


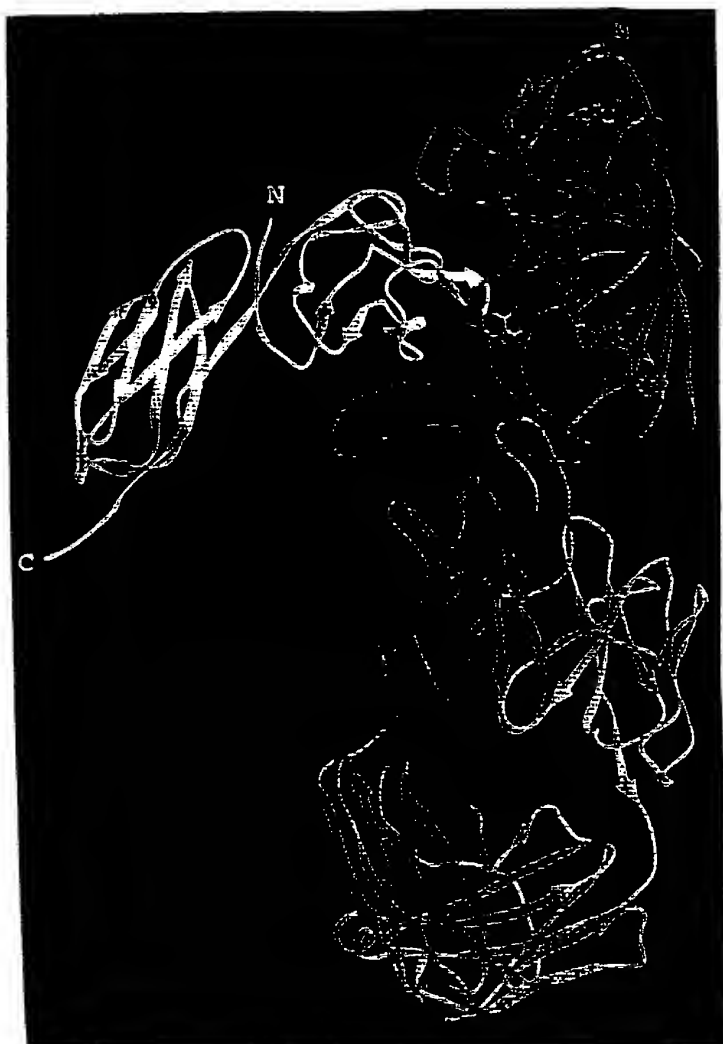
FIG. 27C



FIG. 27D

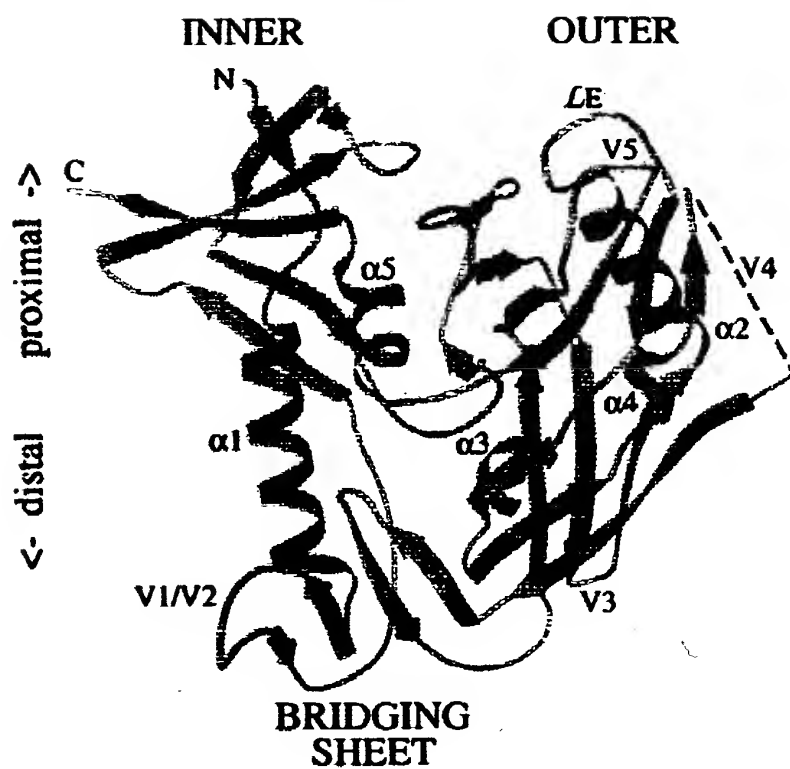
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FIG. 28



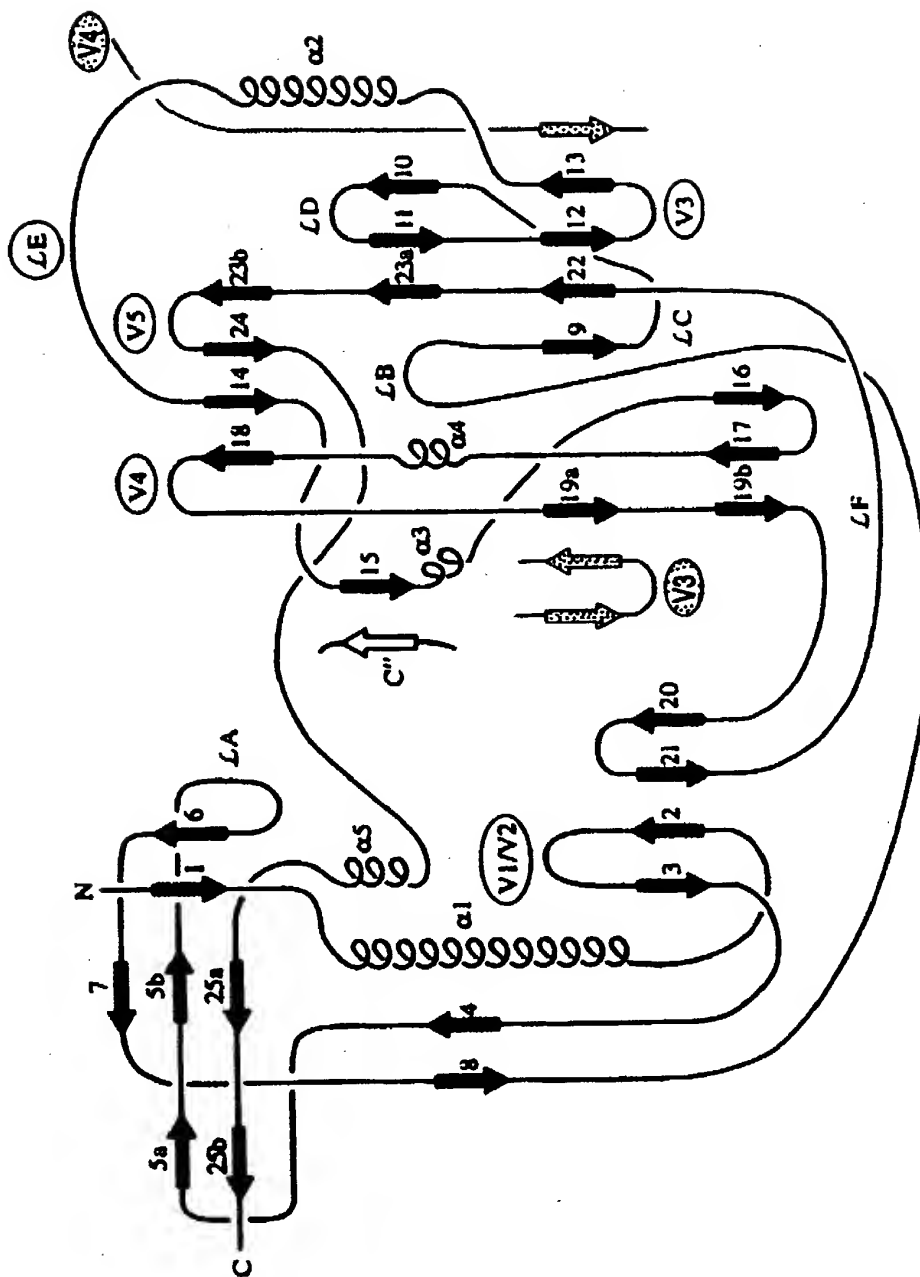
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FIG. 29A



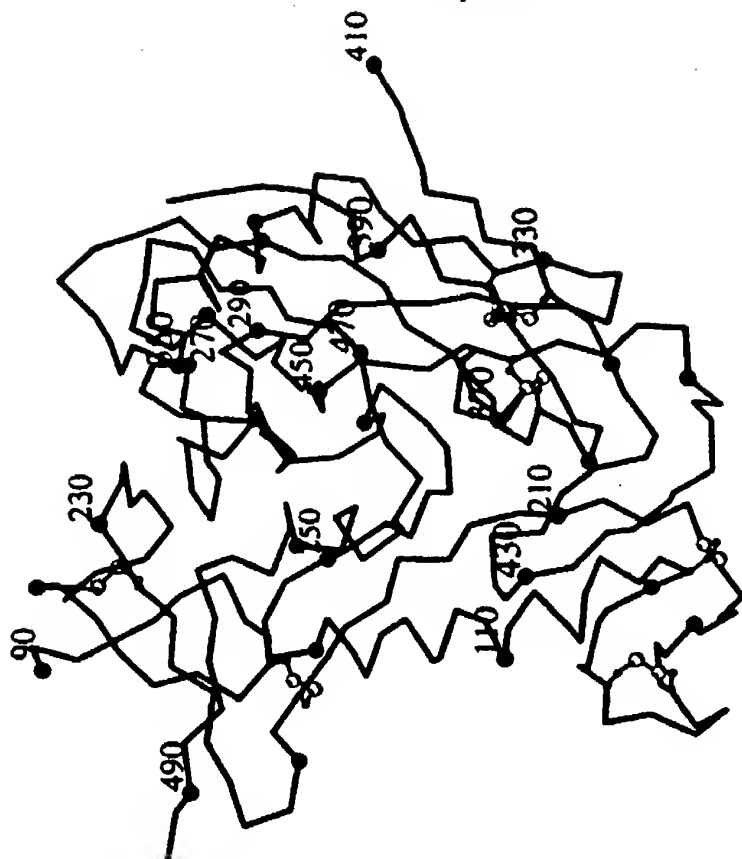
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FIG. 29B



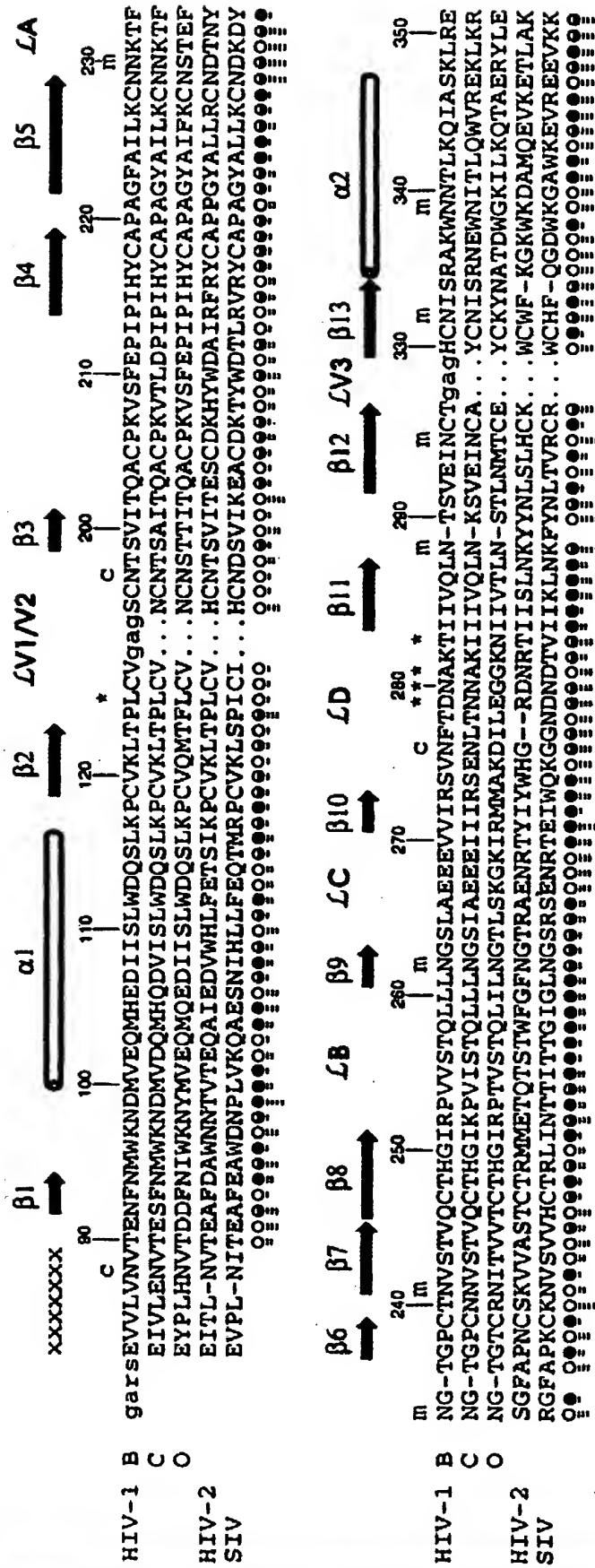
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FIG. 29C



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FIG. 29D-1





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FIG. 30A



FIG. 30B





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FIG. 30F

FIG. 30G

FIG. 30H

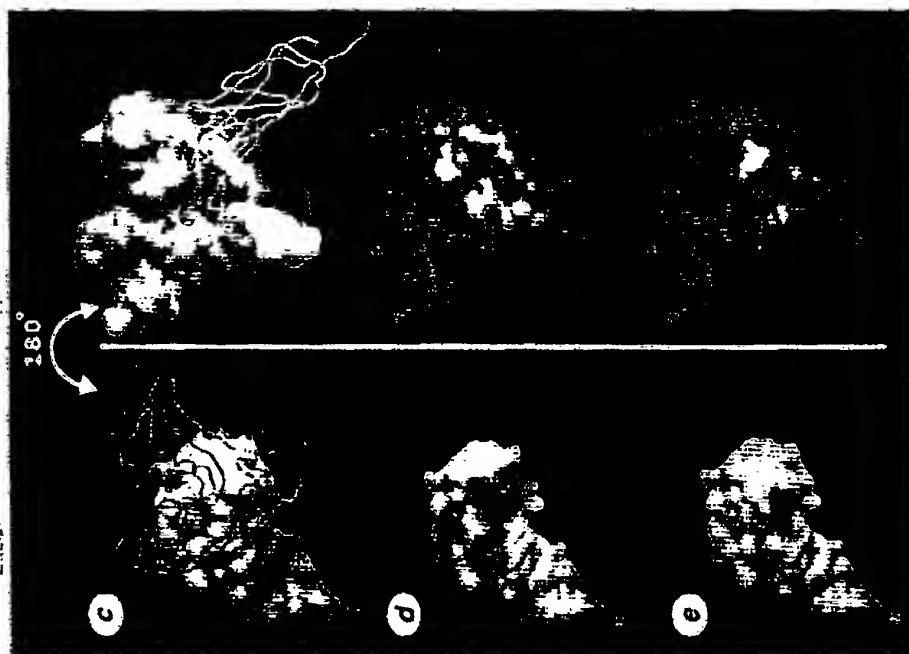
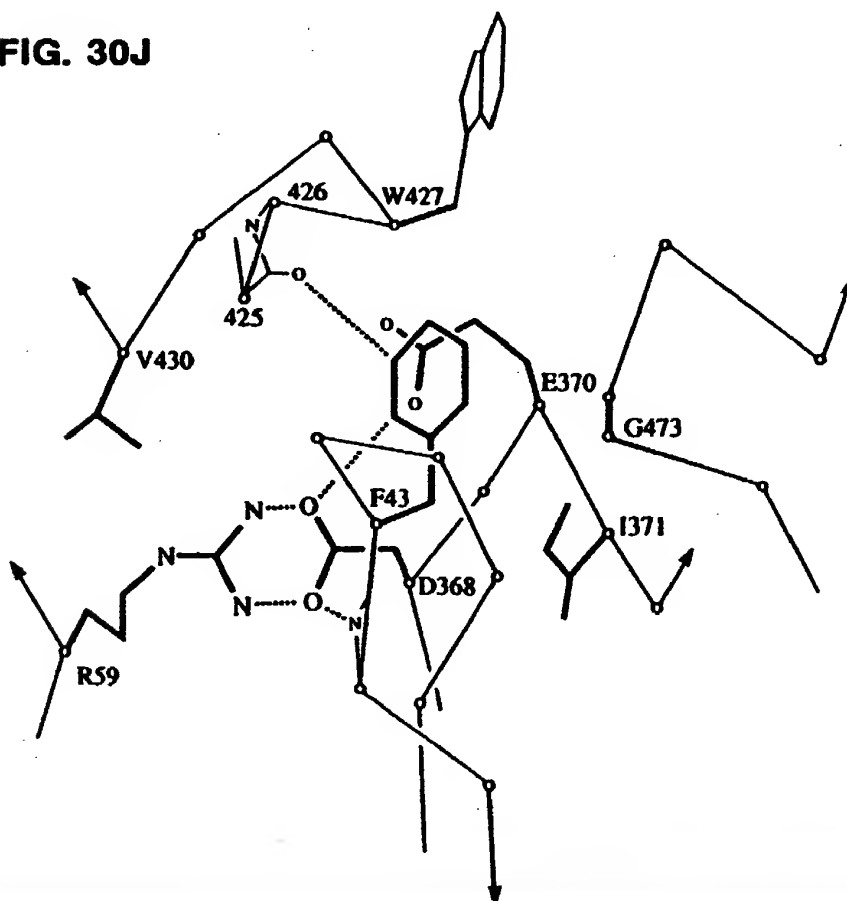


FIG. 30C

FIG. 30D

FIG. 30E



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FIG. 31A



FIG. 31B

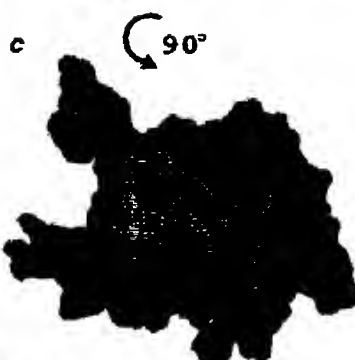
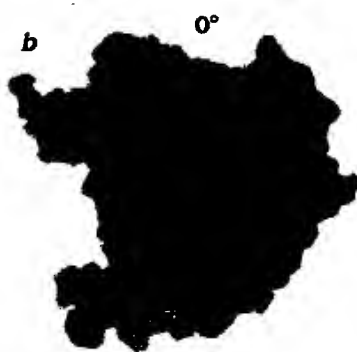


FIG. 31C

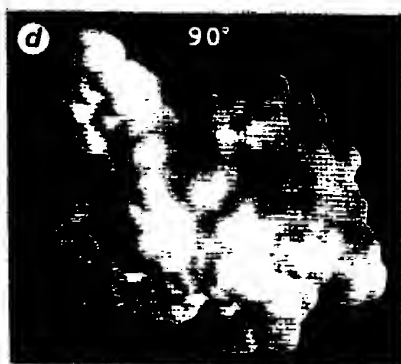


FIG. 31D

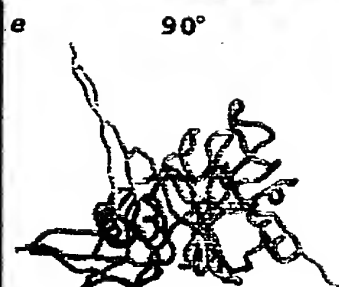
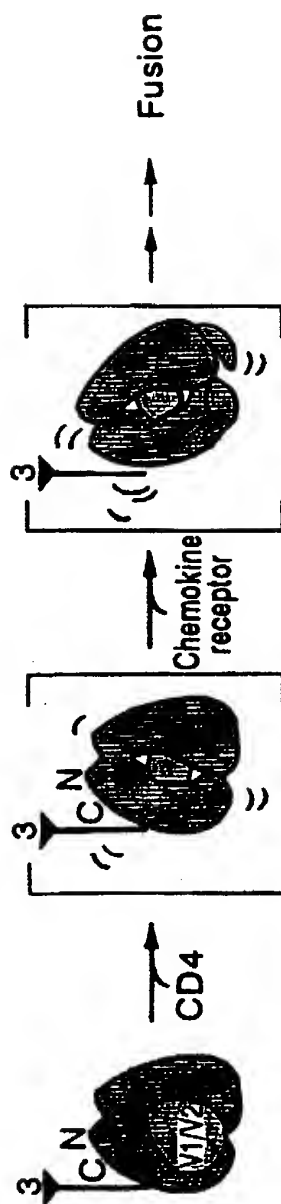


FIG. 31E

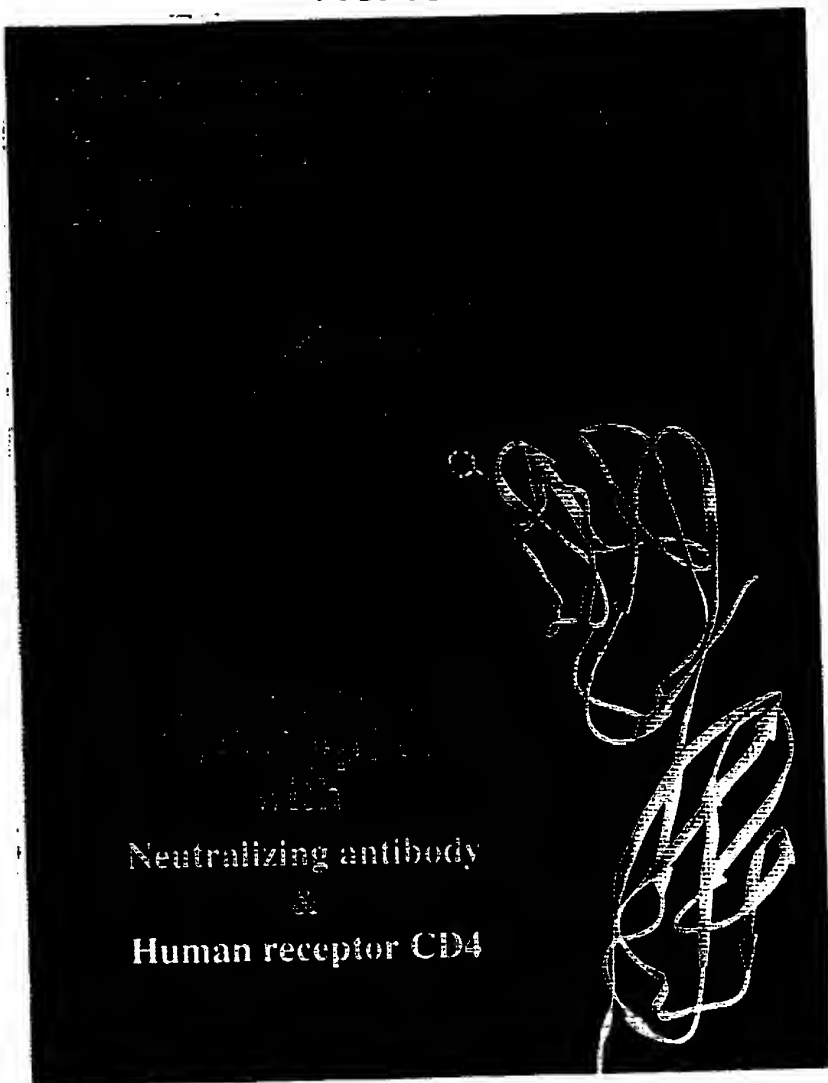
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FIG. 32



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FIG. 33



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FIG. 34A

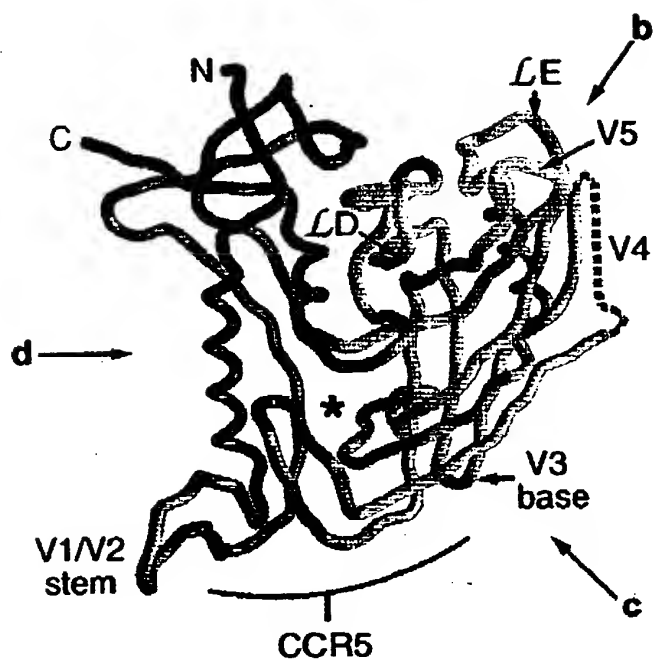


FIG. 34B



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FIG. 34C

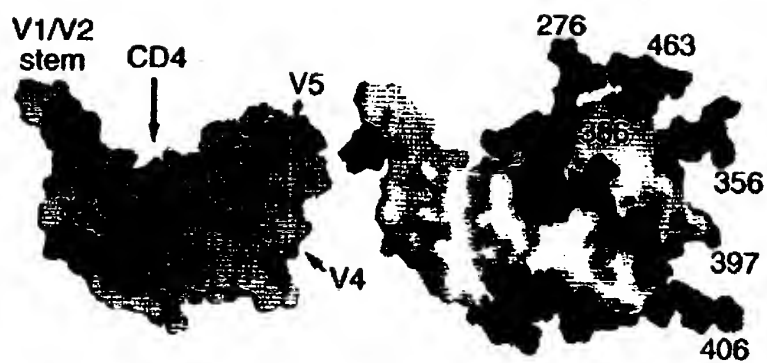
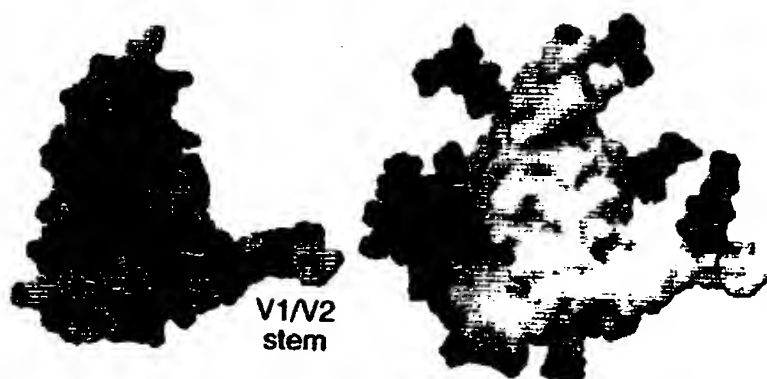
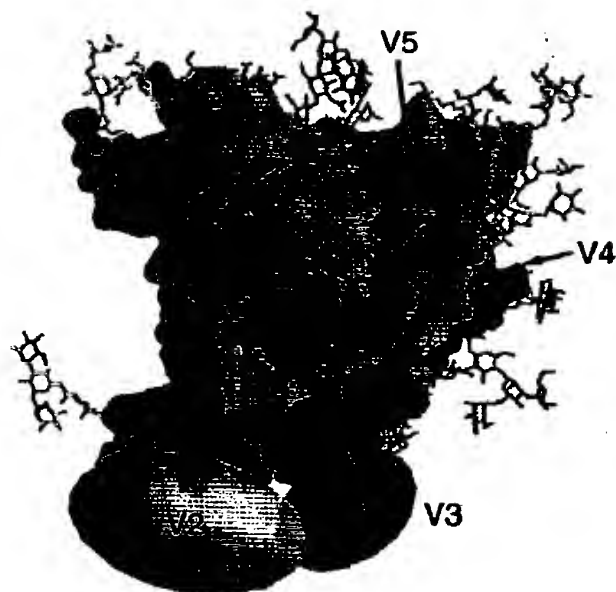


FIG. 34D



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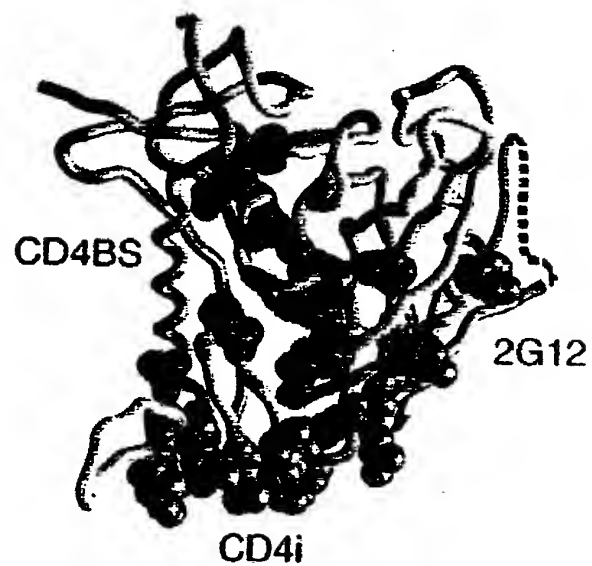
FIG. 35A





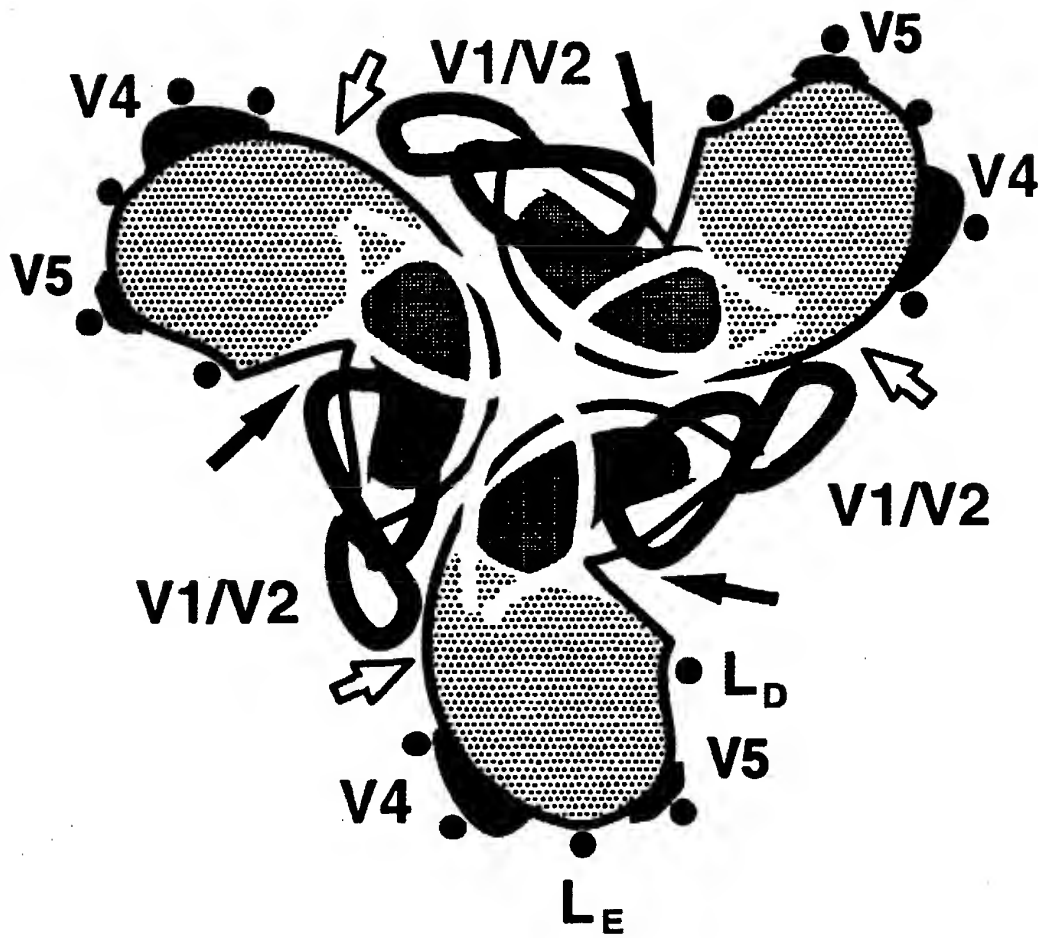
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FIG. 35B



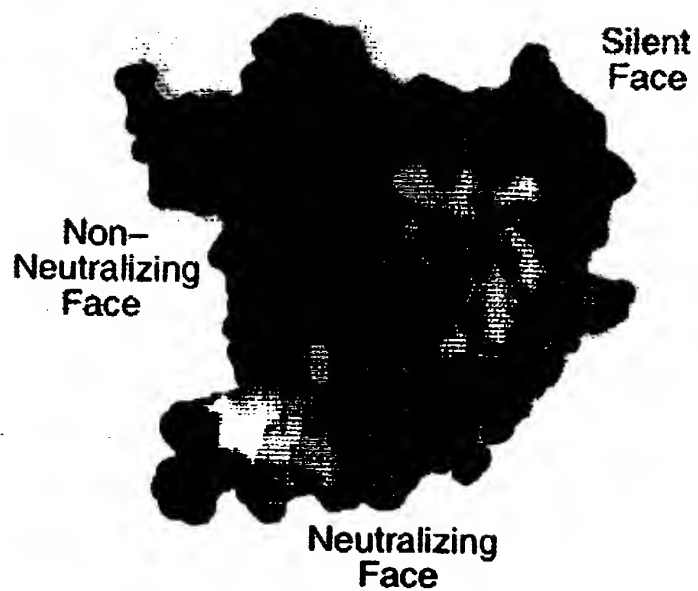
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FIG. 35C



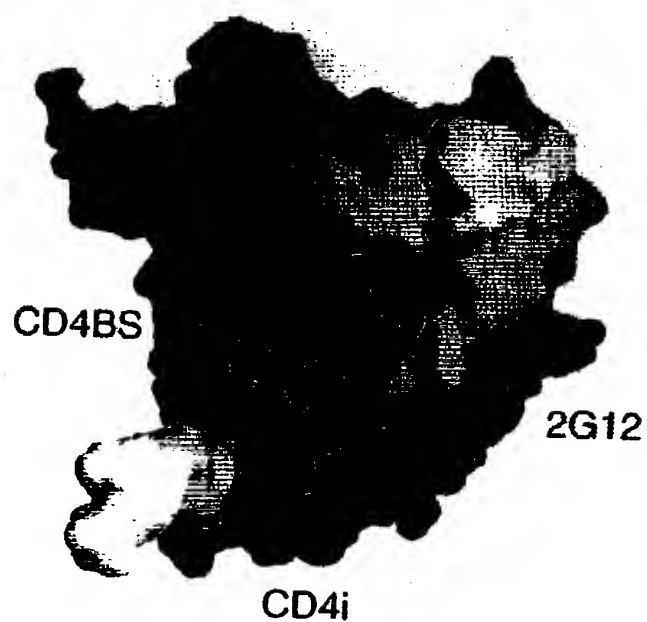
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FIG. 35D



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FIG. 36



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FIG. 37



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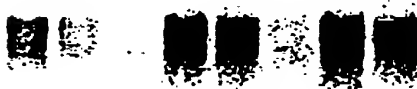
FIG. 38A

L1.2	L1.2-CCR5	L1.2-CCR5
------	-----------	-----------



FIG. 38B

17b μg/ml			MIP-1β ng/ml			2D7 ng/ml		
1	4	10	2	20	200	10 <sup>1</sup>	10 <sup>2</sup>	10 <sup>3</sup>

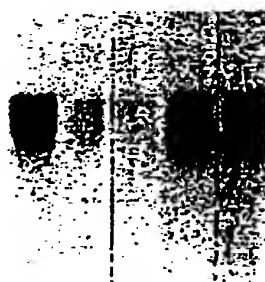


- 200  
- 97  
- 66  
- 46

sCD4 + + -

FIG. 38C

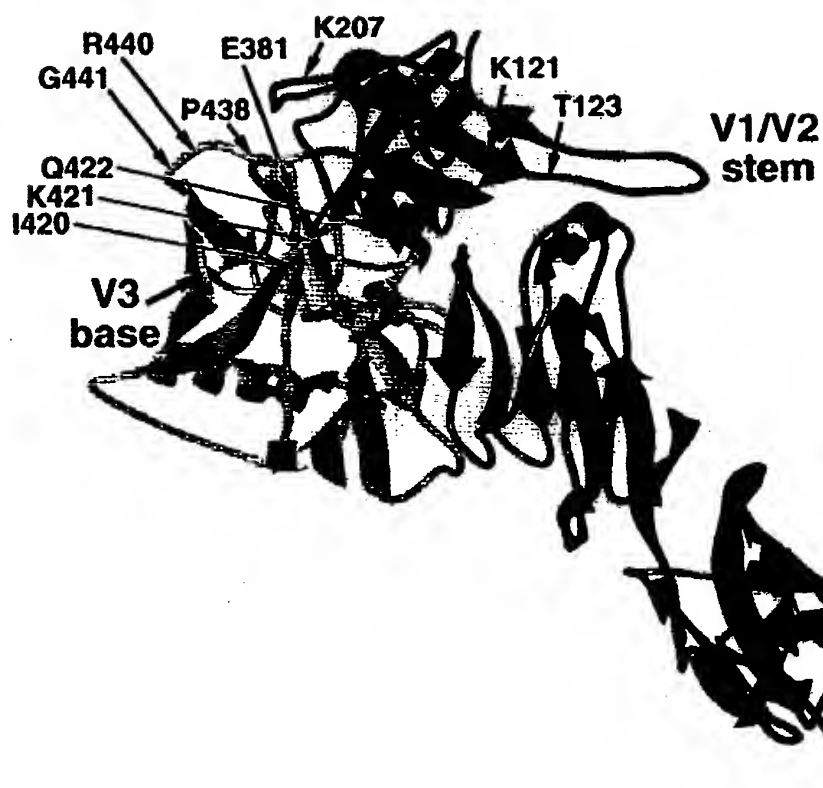
Total					Bound (sCD4)					Bound (CCR5)				
WT	117	121	122	200	WT	117	121	122	200	WT	117	121	122	200
	K/D	K/D	L/S	V/S		K/D	K/D	L/S	V/S		K/D	K/D	L/S	V/S



- 200  
- 97  
- 66  
- 46

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FIG. 39A



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FIG. 39B-1

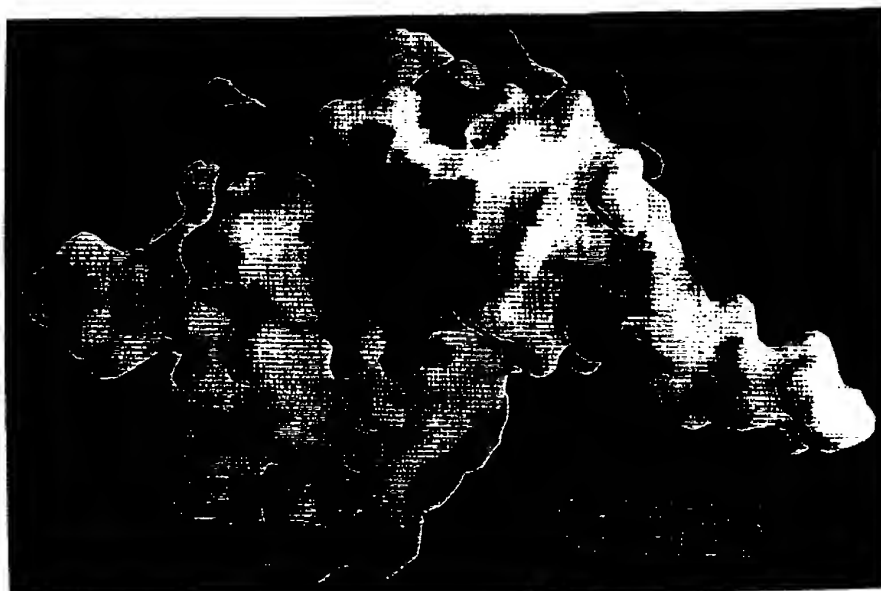
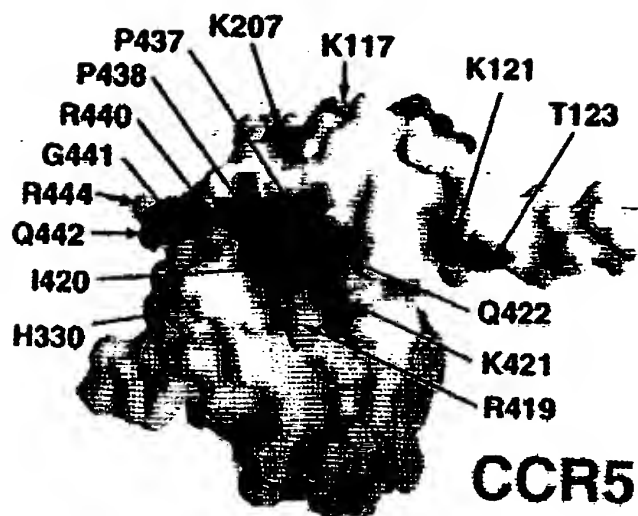


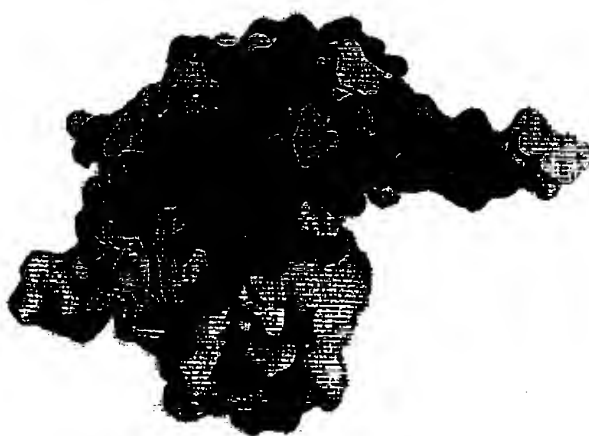
FIG. 39B-2





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FIG. 39C

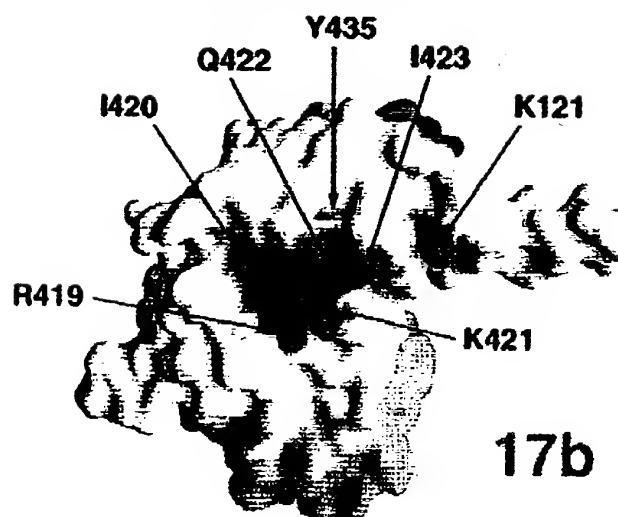


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FIG. 39D-1



FIG. 39D-2



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FIG. 39E-1

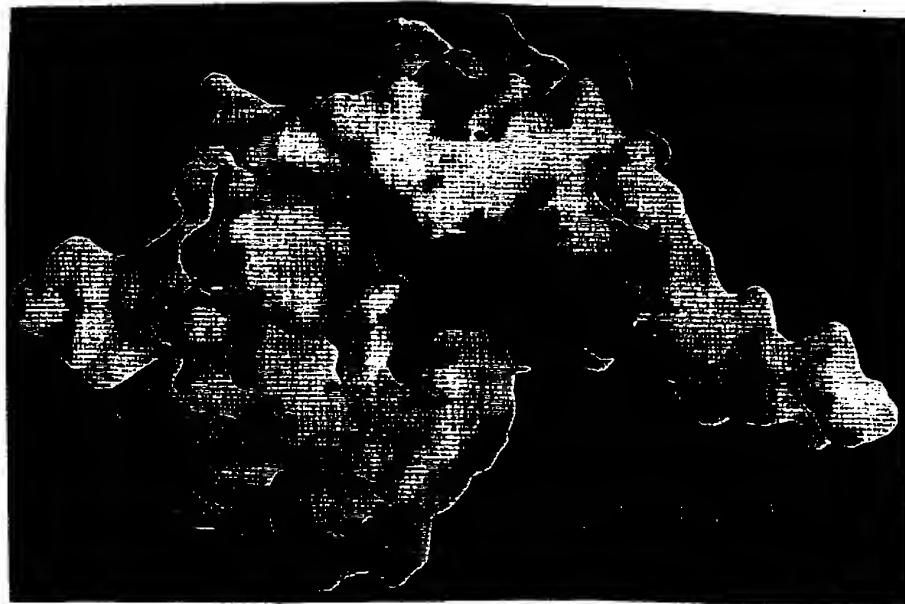
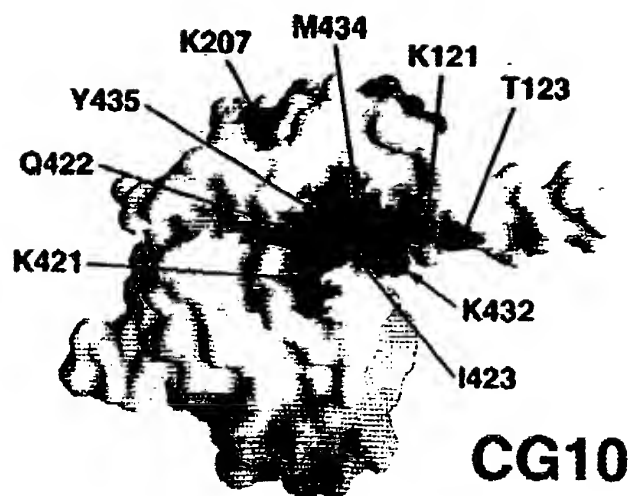
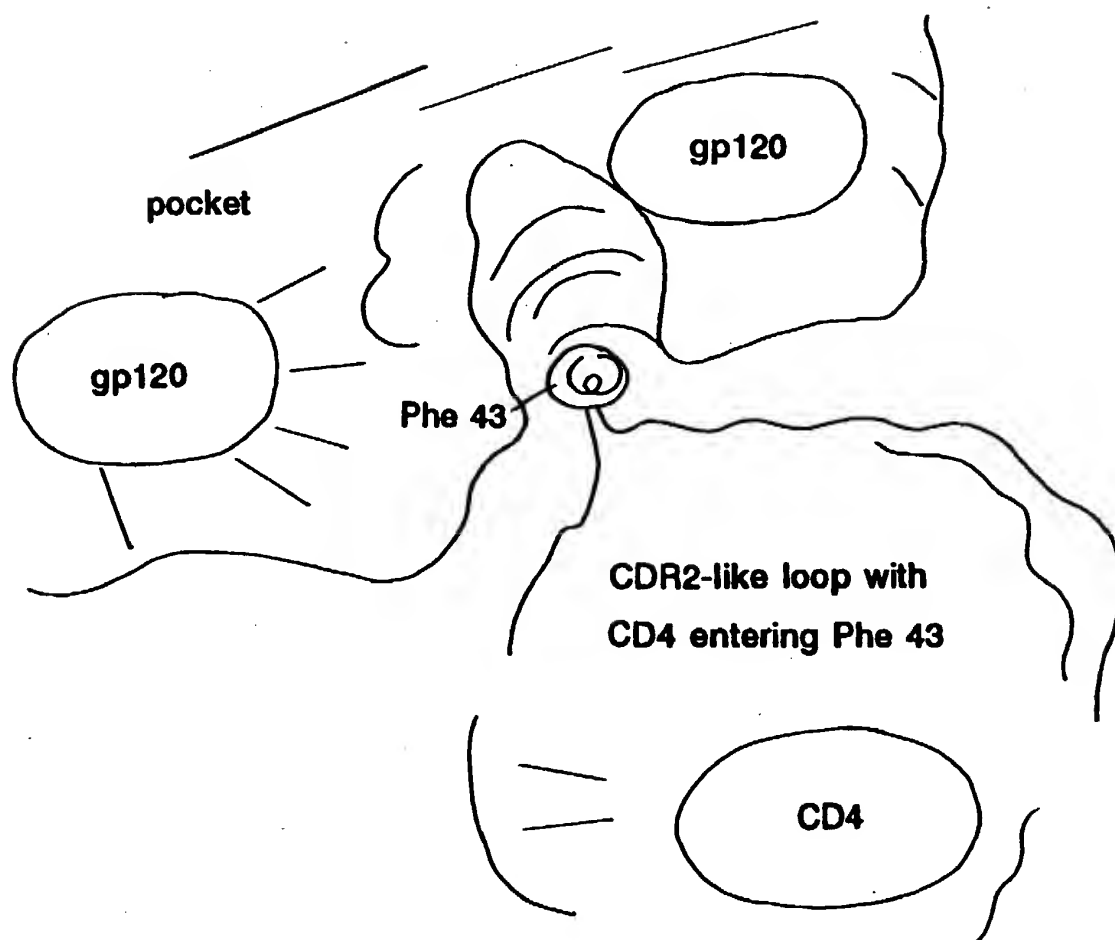


FIG. 39E-2



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FIG. 40



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FIG. 41A

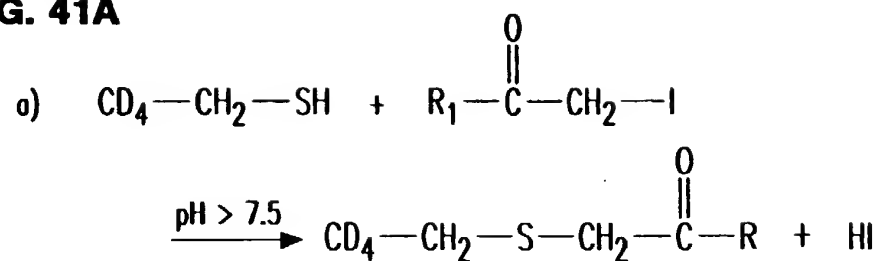
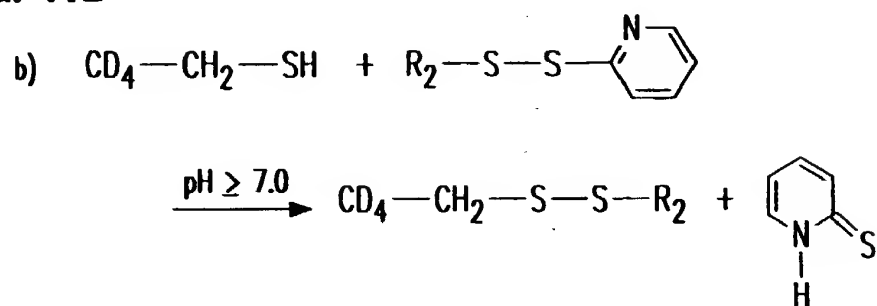
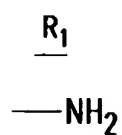
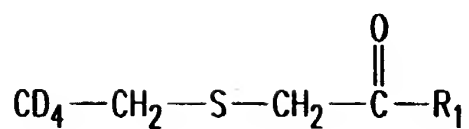


FIG. 41B

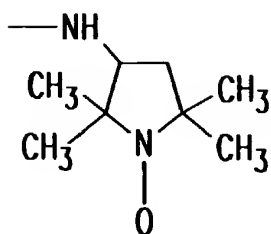


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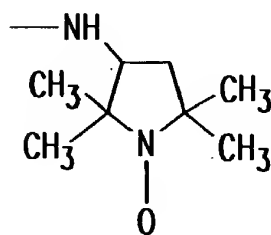
FIG. 42

Reagent

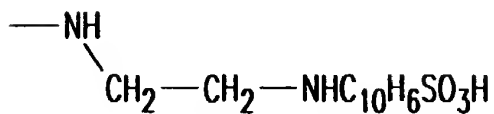
Iodoacetamide



3-(2-Iodoacetamide)-proxyl



4-(2-Iodoacetamide)-tempo



N-Iodoacetyl-N'-(5-sulfonyl-1-naphthyl) ethylene diamine

-or-

N-Iodoacetyl-N'-(8-sulfonyl-1-naphthyl) ethylene diamine

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FIG. 43A



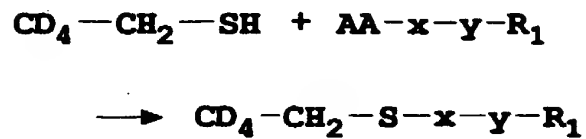
AA = reactive with thiols

BB = reactive with B\*

x = linker

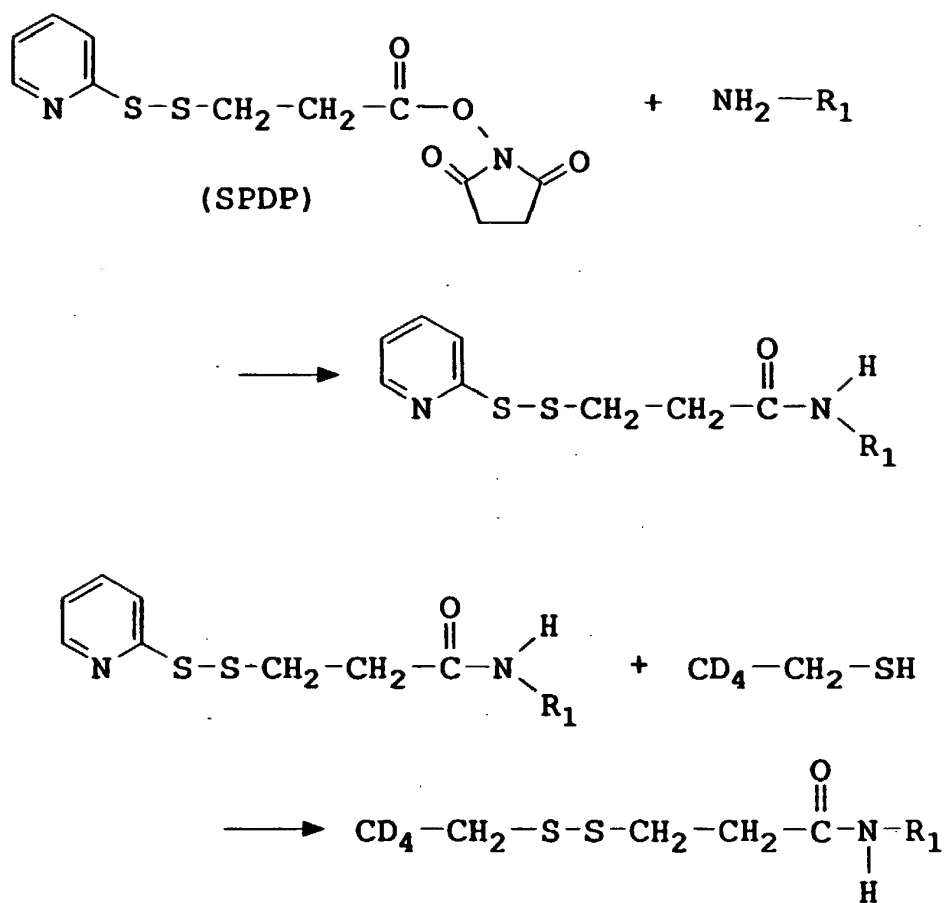
y = result of BB + B\*

FIG. 43B



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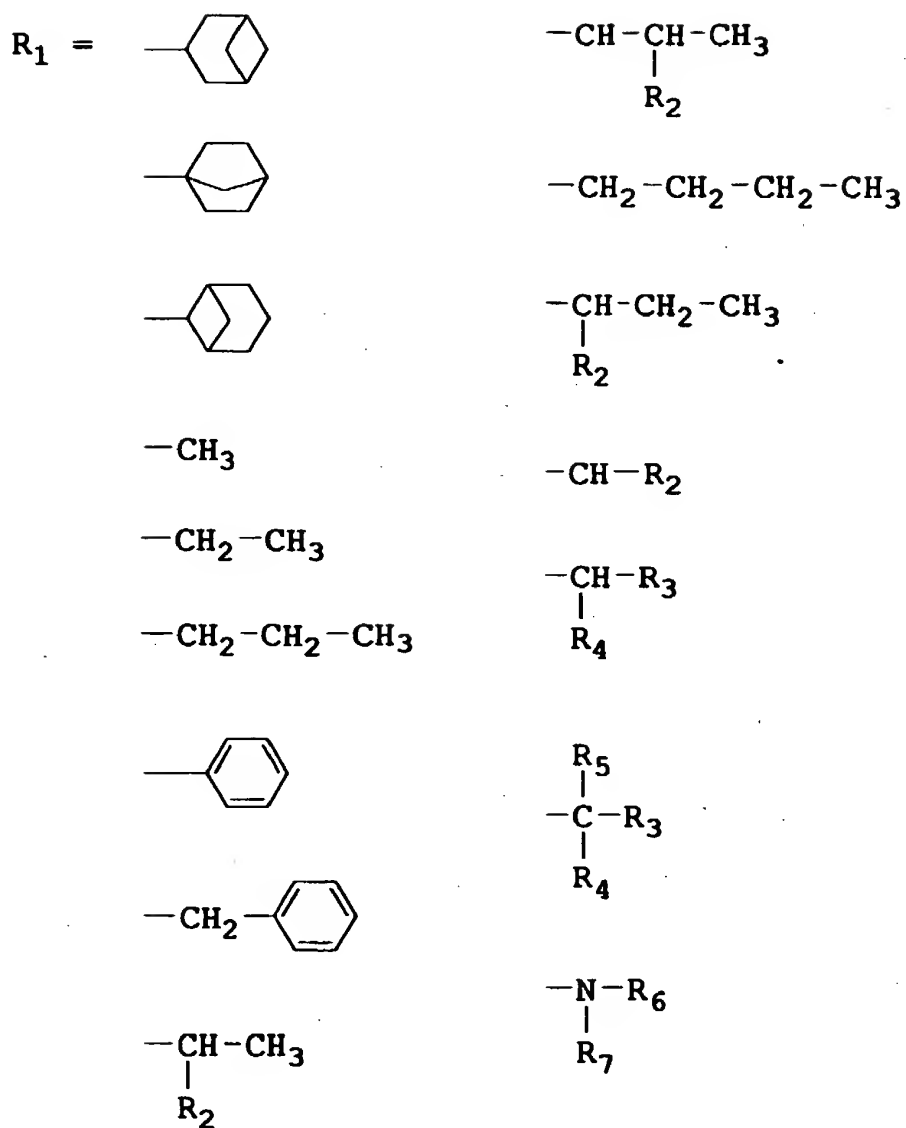
FIG. 44A





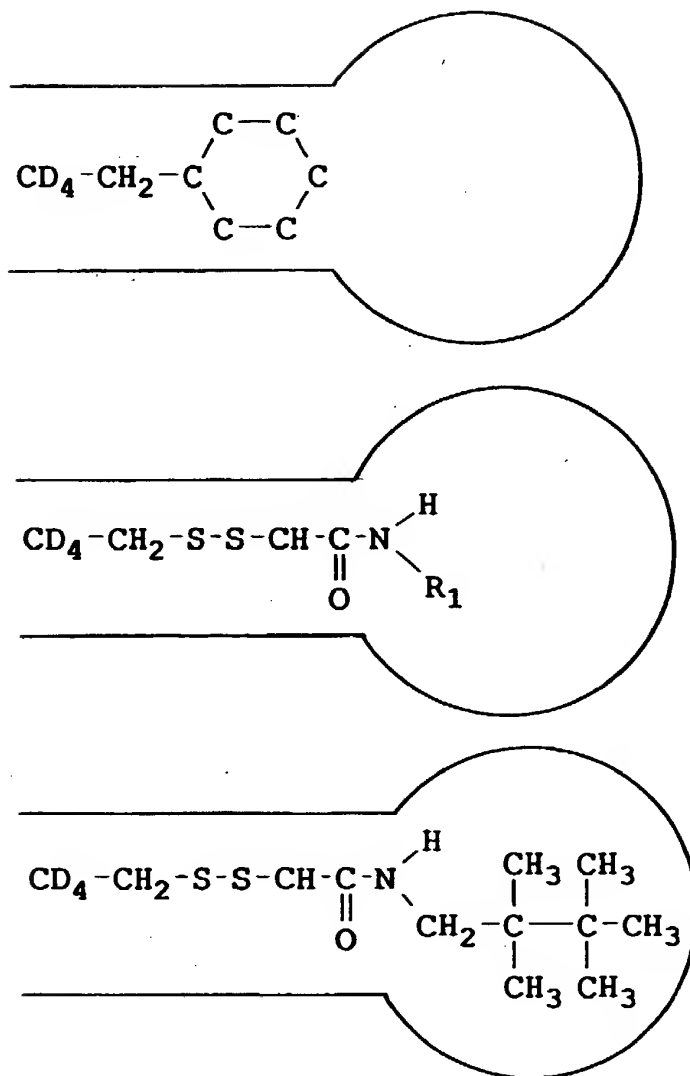
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FIG. 44B



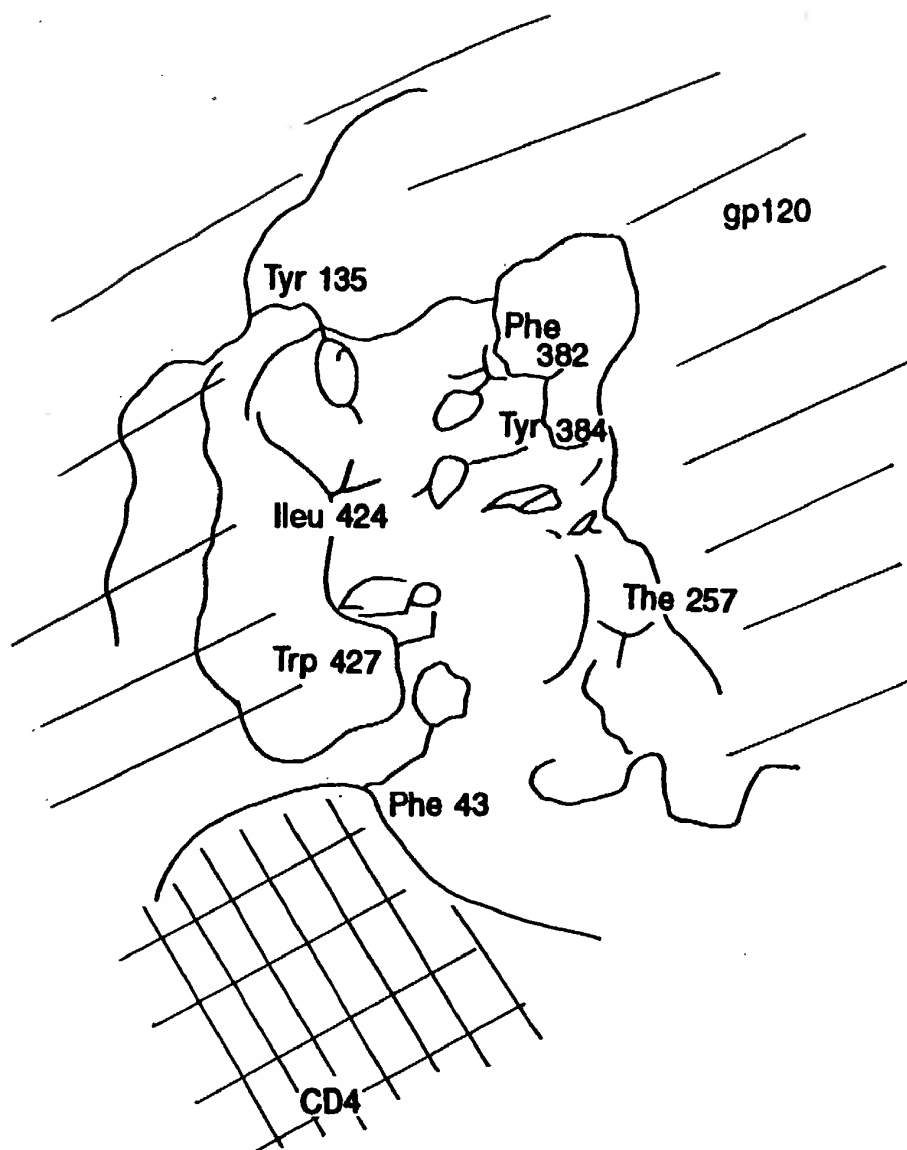
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FIG. 45



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FIG. 46



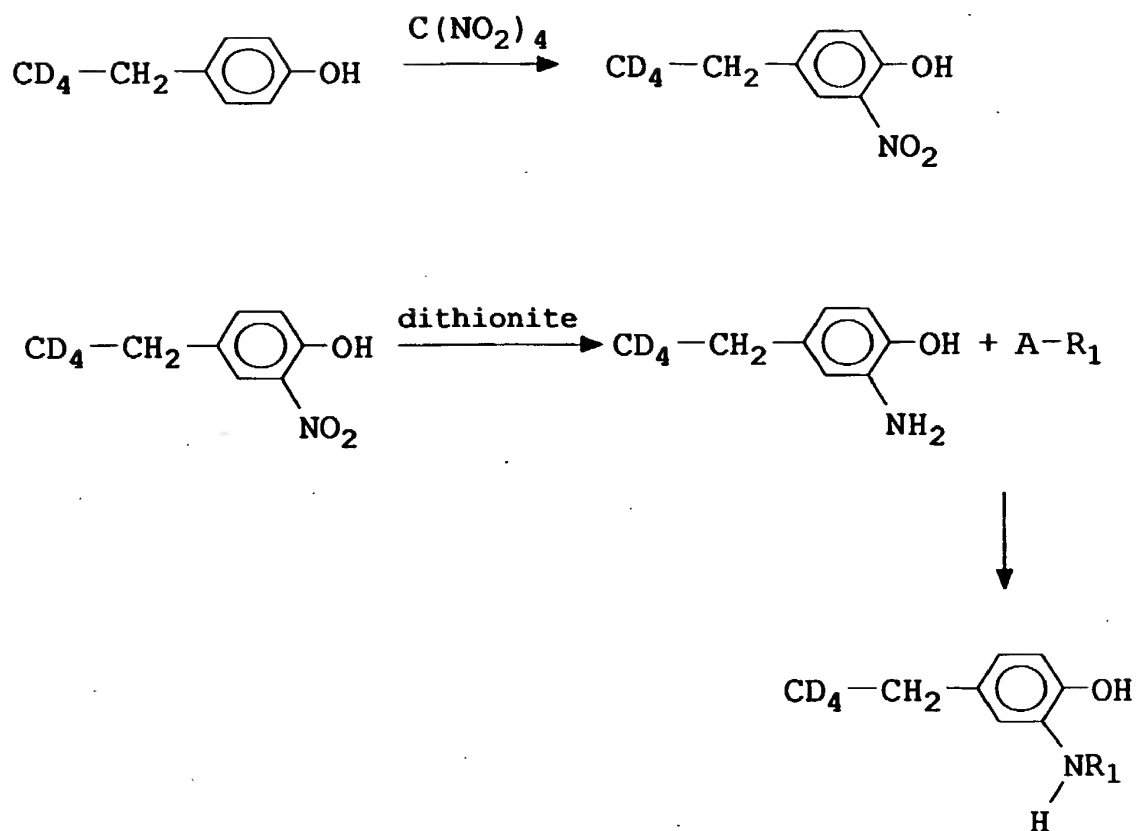
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FIG. 47



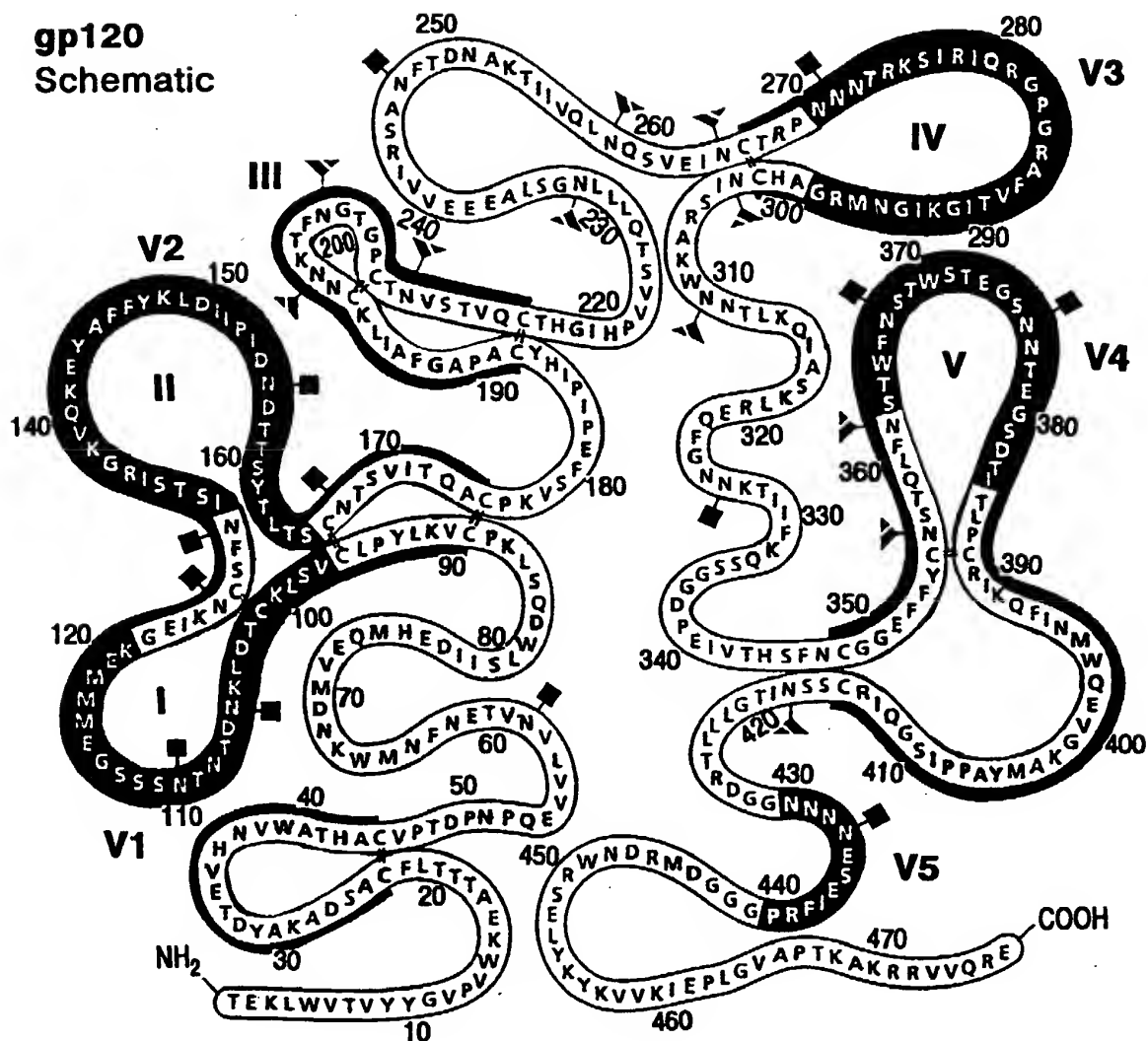
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FIG. 48



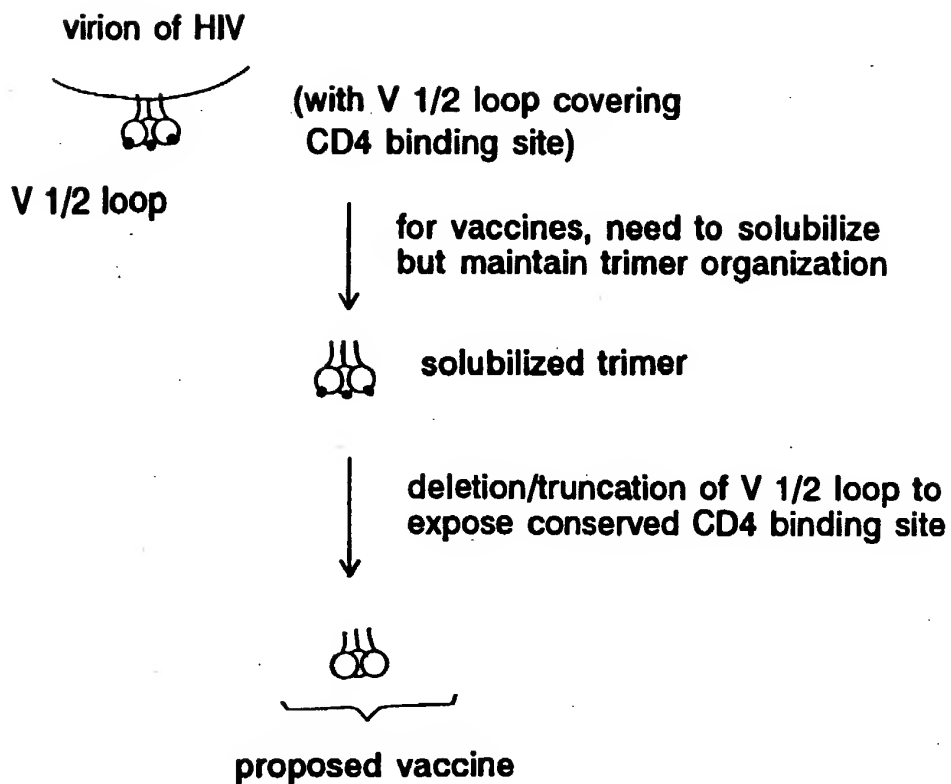
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FIG. 49



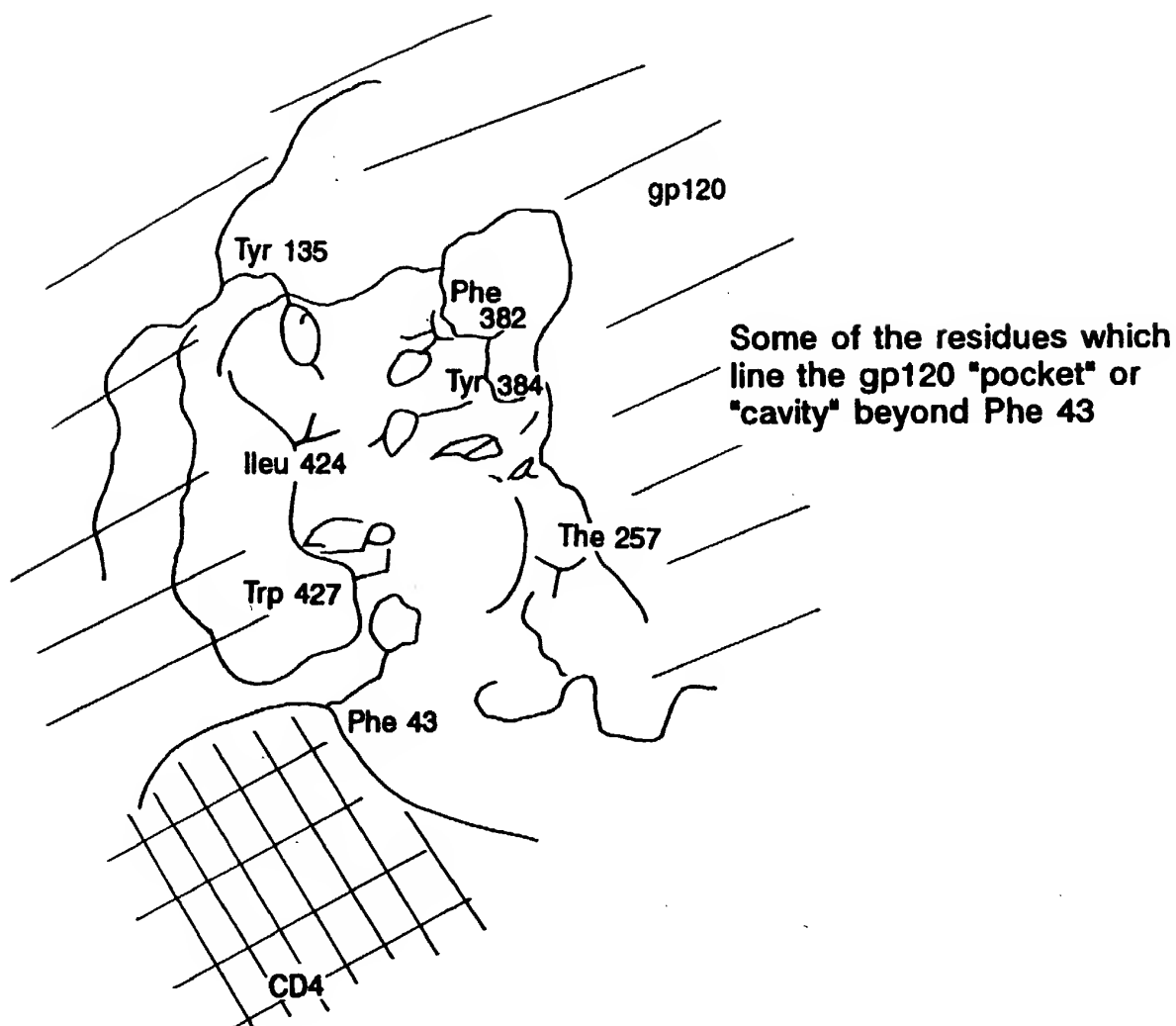
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FIG. 50



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FIG. 51

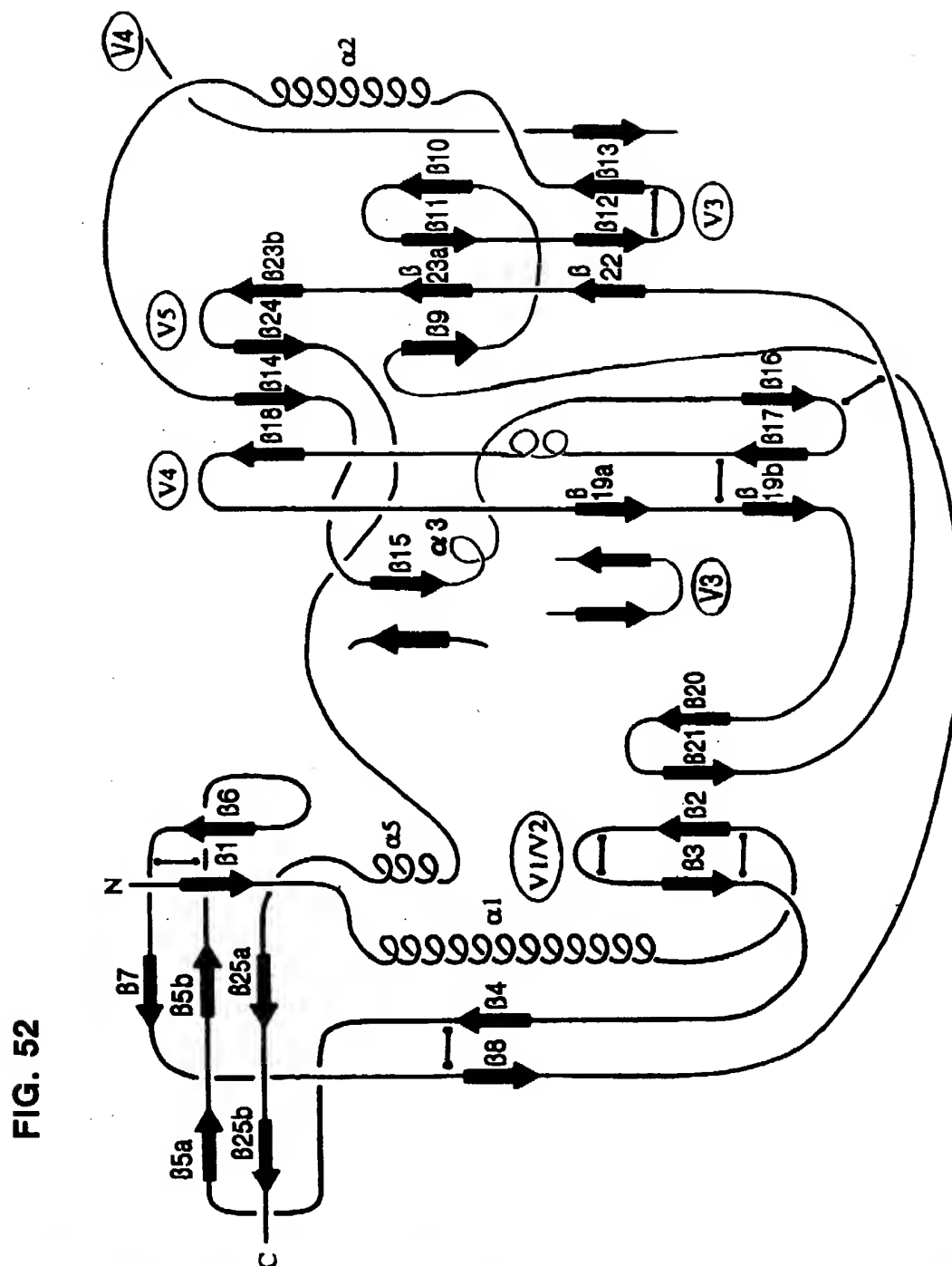


Residues which line the pocket include:

Trp 112	Ser 375	Asn 428
Leu 116	Asn 377	Ala 433
Pro 118	Phe 382	Gly 473
Phe 210	Ileu 424	Met 475
Val 255	Met 426	
Thr 257	Trp 427	



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FIG. 53-1 HEADER COMPLEX (HIV ENVELOPE PROTEIN/CD4/FAB) 15-JUN-98 1GC1  
 TITLE HIV-1 GP120 CORE COMPLEXED WITH CD4 AND A NEUTRALIZING  
 TITLE 2 HUMAN ANTIBODY  
 COMPND MOL ID: 1;  
 COMPND 2 MOLECULE: ENVELOPE PROTEIN GP120;  
 COMPND 3 CHAIN: G;  
 COMPND 4 FRAGMENT: CORE;  
 COMPND 5 ENGINEERED: YES;  
 COMPND 6 MUTATION: (GARS) SUBSTITUTION AT THE N TERMINUS, GLY ALA  
 COMPND 7 GLY SUBSTITUTIONS FOR THE V1/V2 AND V3 LOOPS;  
 COMPND 8 MOL ID: 2;  
 COMPND 9 MOLECULE: CD4;  
 COMPND 10 CHAIN: C;  
 COMPND 11 FRAGMENT: D1D2, N-TERMINAL TWO DOMAIN FRAGMENT;  
 COMPND 12 ENGINEERED: YES;  
 COMPND 13 MUTATION: S184N, I185T;  
 COMPND 14 MOL ID: 3;  
 COMPND 15 MOLECULE: ANTIBODY 17B;  
 COMPND 16 CHAIN: L, H;  
 COMPND 17 FRAGMENT: ANTIGEN-BINDING FRAGMENT, FAB;  
 COMPND 18 ENGINEERED: YES;  
 COMPND 19 OTHER DETAILS: MONOCLONAL ANTIBODY 17B BINDS TO A  
 COMPND 20 CD4-INDUCED SITE ON GP120  
 SOURCE MOL ID: 1;  
 SOURCE 2 ORGANISM SCIENTIFIC: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1;  
 SOURCE 3 ORGANISM COMMON: HIV-1;  
 SOURCE 4 STRAIN: CLADE B;  
 SOURCE 5 VARIANT: HXBC2;  
 SOURCE 6 EXPRESSION SYSTEM: DROSOPHILA MELANOGASTER;  
 SOURCE 7 OTHER DETAILS: SECRETED FROM DROSOPHILA SCHNEIDER 2 LINES  
 SOURCE 8 UNDER CONTROL OF AN INDUCIBLE METALLOTHIONEIN PROMOTER;  
 SOURCE 9 MOL ID: 2;  
 SOURCE 10 ORGANISM SCIENTIFIC: HOMO SAPIENS;  
 SOURCE 11 ORGANISM COMMON: HUMAN;  
 SOURCE 12 EXPRESSION SYSTEM: CHINESE HAMSTER OVARY CELLS (CHO),  
 SOURCE 13 CRICETULUS GRISEUS;  
 SOURCE 14 MOL ID: 3;  
 SOURCE 15 ORGANISM SCIENTIFIC: HOMO SAPIENS;  
 SOURCE 16 ORGANISM COMMON: HUMAN;  
 SOURCE 17 EXPRESSION SYSTEM: EPSTEIN-BARR VIRUS IMMORTALIZED B-CELL  
 SOURCE 18 CLONE FUSED WITH A MURINE B-CELL FUSION PARTNER  
 KEYWDS COMPLEX (HIV ENVELOPE PROTEIN/CD4/FAB), HIV-1 EXTERIOR  
 KEYWDS 2 ENVELOPE GP120, T-CELL SURFACE GLYCOPROTEIN CD4,  
 KEYWDS 3 ANTIGEN-BINDING FRAGMENT OF HUMAN IMMUNOGLOBULIN 17B,  
 KEYWDS 4 GLYCOSYLATED PROTEIN  
 EXPDTA X-RAY DIFFRACTION  
 AUTHOR P.D.KWONG,R.WYATT,J.ROBINSON,R.W.SWEET,J.SODROSKI,  
 AUTHOR 2 W.A.HENDRICKSON  
 REVDAT 2 19-AUG-98 1GC1A 1 SSBOND SOURCE COMPND REMARK  
 REVDAT 21 1 DBREF SEQADV  
 REVDAT 1 08-JUL-98 1GC1 0  
 JRNL AUTH P.D.KWONG,R.WYATT,J.ROBINSON,R.W.SWEET,J.SODROSKI,  
 JRNL AUTH 2 W.A.HENDRICKSON  
 JRNL TITL STRUCTURE OF AN HIV GP120 ENVELOPE GLYCOPROTEIN IN  
 JRNL TITL 2 COMPLEX WITH THE CD4 RECEPTOR AND A NEUTRALIZING  
 JRNL TITL 3 HUMAN ANTIBODY  
 JRNL REF NATURE V. 393 648 1998  
 JRNL REFN ASTM NATUAS UK ISSN 0028-0836 0006  
 REMARK 1  
 REMARK 2  
 REMARK 2 RESOLUTION. 2.5 ANGSTROMS.  
 REMARK 3  
 REMARK 3 REFINEMENT.  
 REMARK 3 PROGRAM : X-PLOR 3.8  
 REMARK 3 AUTHORS : BRUNGER  
 REMARK 3  
 REMARK 3 DATA USED IN REFINEMENT.  
 REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.5  
 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 5  
 REMARK 3 DATA CUTOFF (SIGMA(F)) : 2

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FIG. 53-2

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REMARK 3 DATA CUTOFF LOW (ABS(F)) : 0.1
REMARK 3 COMPLETENESS (WORKING+TEST) (%) : 74.9
REMARK 3 NUMBER OF REFLECTIONS : 28620
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING SET) : 0.2103
REMARK 3 FREE R VALUE : 0.3026
REMARK 3 FREE R VALUE TEST SET SIZE (%) : 5
REMARK 3 FREE R VALUE TEST SET COUNT : 1430
REMARK 3 ESTIMATED ERROR OF FREE R VALUE : NULL
REMARK 3
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK 3 TOTAL NUMBER OF BINS USED : 10
REMARK 3 BIN RESOLUTION RANGE HIGH (A) : 2.50
REMARK 3 BIN RESOLUTION RANGE LOW (A) : 2.58
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 42.3
REMARK 3 REFLECTIONS IN BIN (WORKING SET) : 1518
REMARK 3 BIN R VALUE (WORKING SET) : 0.2876
REMARK 3 BIN FREE R VALUE : 0.3878
REMARK 3 BIN FREE R VALUE TEST SET SIZE (%) : 5.7
REMARK 3 BIN FREE R VALUE TEST SET COUNT : 92
REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : NULL
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 7080
REMARK 3 NUCLEIC ACID ATOMS : 0
REMARK 3 HETEROGEN ATOMS : 194
REMARK 3 SOLVENT ATOMS : 602
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : NULL
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 21
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : 0
REMARK 3 B22 (A**2) : 0
REMARK 3 B33 (A**2) : 0
REMARK 3 B12 (A**2) : 0
REMARK 3 B13 (A**2) : 0
REMARK 3 B23 (A**2) : 0
REMARK 3
REMARK 3 ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM LUZZATI PLOT (A) : NULL
REMARK 3 ESD FROM SIGMAA (A) : NULL
REMARK 3 LOW RESOLUTION CUTOFF (A) : 5.0
REMARK 3
REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM C-V LUZZATI PLOT (A) : NULL
REMARK 3 ESD FROM C-V SIGMAA (A) : NULL
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3 BOND LENGTHS (A) : 0.007
REMARK 3 BOND ANGLES (DEGREES) : 1.59
REMARK 3 DIHEDRAL ANGLES (DEGREES) : NULL
REMARK 3 IMPROPER ANGLES (DEGREES) : NULL
REMARK 3
REMARK 3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. RMS SIGMA
REMARK 3 MAIN-CHAIN BOND (A**2) : 1.33 ; 1.0
REMARK 3 MAIN-CHAIN ANGLE (A**2) : 2.31 ; 1.5
REMARK 3 SIDE-CHAIN BOND (A**2) : 1.97 ; 1.5
REMARK 3 SIDE-CHAIN ANGLE (A**2) : 3.01 ; 2.0
REMARK 3
REMARK 3 NCS MODEL : NULL
REMARK 3
REMARK 3 NCS RESTRAINTS. RMS SIGMA/WEIGHT
REMARK 3 GROUP 1 POSITIONAL (A) : NULL ; NULL
REMARK 3 GROUP 1 FACTOR (A**2) : NULL ; NULL

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FIG. 53-3

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REMARK 3 PARAMETER FILE 1 : PARAM3 MOD.CHO
REMARK 3 PARAMETER FILE 2 : PARAMCSDX.MISC
REMARK 3 PARAMETER FILE 3 : PARAMCSDX MOD.PRO
REMARK 3 PARAMETER FILE 4 : PARAM19.SOL
REMARK 3 TOPOLOGY FILE 1 : TOPHCSDX.PRO
REMARK 3 TOPOLOGY FILE 2 : TOPH3.CHO
REMARK 3 TOPOLOGY FILE 3 : TOPHCSDX.MISC
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: NULL
REMARK 4
REMARK 4 1GC1 COMPLIES WITH FORMAT V. 2.2, 16-DEC-1996
REMARK 6
REMARK 6 RESIDUES 83-89 AND 397-409 OF GP120 AND 182-185 OF CD4 ARE
REMARK 6 DISORDERED AND ARE IN SEQUENCE LIST BUT NOT IN ATOMS LIST.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : AUG-1996
REMARK 200 TEMPERATURE (KELVIN): 100
REMARK 200 PH : 7.0
REMARK 200 NUMBER OF CRYSTALS USED : 1
REMARK 200
REMARK 200 SYNCHROTRON (Y/N): Y
REMARK 200 RADIATION SOURCE : NSLS
REMARK 200 BEAMLINE : X4A
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L): M
REMARK 200 WAVELENGTH OR RANGE (A): 1.00614
REMARK 200 MONOCHROMATOR : SILICON CRYSTAL
REMARK 200 OPTICS : MIRRORS
REMARK 200
REMARK 200 DETECTOR TYPE : PHOSPHOR IMAGE PLATE
REMARK 200 FUJI BAS2000 SCANNER
REMARK 200 DETECTOR MANUFACTURER : FUJI
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE : SCALEPACK
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 37724
REMARK 200 RESOLUTION RANGE HIGH (A): 2.5
REMARK 200 RESOLUTION RANGE LOW (A): 20.
REMARK 200 REJECTION CRITERIA (SIGMA(I)): -0.5
REMARK 200
REMARK 200 OVERALL
REMARK 200 COMPLETENESS FOR RANGE (%): 86
REMARK 200 DATA REDUNDANCY : 3.0
REMARK 200 R MERGE (I): NULL
REMARK 200 R SYM (I): 0.093
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 9.17
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A): 2.50
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.59
REMARK 200 COMPLETENESS FOR SHELL (%): 62.8
REMARK 200 DATA REDUNDANCY IN SHELL : 1.56
REMARK 200 R MERGE FOR SHELL (I): NULL
REMARK 200 R SYM FOR SHELL (I): 0.247
REMARK 200 <I/SIGMA(I)> FOR SHELL : 2.17
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: NULL
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR
REMARK 200 REPLACEMENT + MULTIPLE ISOMORPHOUS REPLACEMENT + DENSITY
REMARK 200 MODIFICATION
REMARK 200 SOFTWARE USED: MERLOT, AMORE, MLPHARE, DM, PRISM
REMARK 200 STARTING MODEL: PDB ENTRIES 1HIL, 1CDH AND 3CD4
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): 59
REMARK 280 MATTHEWS COEFFICIENT VM (ANGSTROMS**3/DA): 3.00

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**FIG. 53-4** REMARK 280 CRYSTALLIZATION CONDITIONS: VAPOUR DIFFUSION  
 REMARK 280 CRYSTALLIZATION: 0.5 UL OF PROTEIN  
 REMARK 280 (~10MG/ML IN 350 MM NACL, 5 MM TRISCL PH 7.0) + 0.4 UL OF  
 REMARK 280 0.1 M NACITRATE, 0.02 M NAHEPES, 10% ISOPROPANOL, 10.5%  
 REMARK 280 MONOMETHYL-PEG 5000, 0.0075% SEAPREP AGAROSE, PH 6.4 OVER  
 REMARK 280 A RESERVOIR OF 0.35 M NACL, 0.1 M NACITRATE, 0.02 M  
 REMARK 280 NAHEPES, 10% ISOPROPANOL, 10.5% MONOMETHYL-PEG 5000,  
 REMARK 280 PH 6.4  
 REMARK 290  
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY  
 REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 2 2 2 1  
 REMARK 290  
 REMARK 290 SYMOP SYMMETRY  
 REMARK 290 NNNMMM OPERATOR  
 REMARK 290 1555 X,Y,Z  
 REMARK 290 2555 -X,-Y,1/2+Z  
 REMARK 290 3555 -X,Y,1/2-Z  
 REMARK 290 4555 X,-Y,-Z  
 REMARK 290  
 REMARK 290 WHERE NNN -> OPERATOR NUMBER  
 REMARK 290 MMM -> TRANSLATION VECTOR  
 REMARK 290  
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS  
 REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM  
 REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY  
 REMARK 290 RELATED MOLECULES.  
 REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000 0.00000  
 REMARK 290 SMTRY2 1 0.000000 1.000000 0.000000 0.00000  
 REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 0.00000  
 REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 0.00000  
 REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000 0.00000  
 REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 98.34776  
 REMARK 290 SMTRY1 3 -1.000000 0.000000 0.000000 0.00000  
 REMARK 290 SMTRY2 3 0.000000 1.000000 0.000000 0.00000  
 REMARK 290 SMTRY3 3 0.000000 0.000000 -1.000000 98.34776  
 REMARK 290 SMTRY1 4 1.000000 0.000000 0.000000 0.00000  
 REMARK 290 SMTRY2 4 0.000000 -1.000000 0.000000 0.00000  
 REMARK 290 SMTRY3 4 0.000000 0.000000 -1.000000 0.00000  
 REMARK 290  
 REMARK 290 REMARK: NULL  
 REMARK 650  
 REMARK 650 HELIX  
 REMARK 650 DETERMINATION METHOD: AUTHOR-DETERMINED + KABSCH AND SANDER  
 REMARK 650 ALGORITHM  
 REMARK 700  
 REMARK 700 SHEET  
 REMARK 700 DETERMINATION METHOD: AUTHOR-DETERMINED + KABSCH AND SANDER  
 REMARK 700 ALGORITHM  
 REMARK 700 SHEET G CONTAINS INTERMOLECULAR HYDROGEN BONDING  
 REMARK 700 (STRAND #15 OF CORE GP120 TO STRAND C\* OF CD4).  
 REMARK 800  
 REMARK 800 SITE  
 REMARK 800 SITE IDENTIFIER: O  
 REMARK 800 SITE DESCRIPTION: WATER HOH 1000 (ZERO OCCUPANCY) MARKS  
 REMARK 800 THE LOCATION OF THE CENTRAL UNMODELLED DENSITY IN THE  
 REMARK 800 "PHE 43" CAVITY.  
 REMARK 999  
 REMARK 999 SEQUENCE  
 REMARK 999 1GC1 G SWS P04578 1 - 89 NOT IN ATOMS LIST  
 REMARK 999 1GC1 G SWS P04578 397 - 409 NOT IN ATOMS LIST  
 REMARK 999 1GC1 G SWS P04578 493 - 856 NOT IN ATOMS LIST  
 REMARK 999 1GC1 C SWS P01730 1 - 25 NOT IN ATOMS LIST  
 REMARK 999 1GC1 C SWS P01730 207 - 458 NOT IN ATOMS LIST  
 REMARK 999  
 REMARK 999 REFERENCE: THE INSERTED RESIDUES GARS AT THE N-TERMINUS OF  
 REMARK 999 THE GP120 SEQUENCE AND NT AT THE C-TERMINUS OF CD4 ARE  
 REMARK 999 CLONING ARTIFACTS. GP120: G 128, A 129, G 194 SUBSTITUTE  
 REMARK 999 FOR THE V1/V2 LOOP (128-194), G 298, A 299, G 329  
 REMARK 999 SUBSTITUTE FOR V3 LOOP (298-329).  
 DATA END

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FIG. 53-5 REMARK 999 BEEN CORRECTED IN THIS PDB ENTRY: D94N, D346A, L470P.  
 REMARK 999 THE 17B ANTIBODY SEQUENCE WAS DETERMINED DURING THE COURSE  
 REMARK 999 OF THE STRUCTURE DETERMINATION AND HAS NOT YET BEEN  
 REMARK 999 DEPOSITED IN ANY SEQUENCE DATA BANK (PERSONAL  
 REMARK 999 COMMUNICATION, RICHARD WYATT).

DBREF 1GC1 G 90 127 SWS P04578 ENV HV1H2 90 127  
 DBREF 1GC1 G 128 194 PDB 1GC1 1GC1 128 194  
 DBREF 1GC1 G 195 297 SWS P04578 ENV HV1H2 195 297  
 DBREF 1GC1 G 298 329 PDB 1GC1 1GC1 298 329  
 DBREF 1GC1 G 330 396 SWS P04578 ENV HV1H2 330 396  
 DBREF 1GC1 G 410 492 SWS P04578 ENV HV1H2 410 492  
 DBREF 1GC1 C 1 181 SWS P01730 CD4 HUMAN 26 206  
 DBREF 1GC1 L 1 213 PDB 1GC1 1GC1 1 213  
 DBREF 1GC1 H 1 229 PDB 1GC1 1GC1 1 229

SEQADV 1GC1 ASN G 94 SWS P04578 ASP 94 CONFLICT  
 SEQADV 1GC1 ALA G 346 SWS P04578 ASP 346 CONFLICT  
 SEQADV 1GC1 G SWS P04578 ASN 397 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 SER 398 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 THR 399 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 TRP 400 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 SER 401 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 THR 402 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 GLU 403 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 GLY 404 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 SER 405 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 ASN 406 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 ASN 407 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 THR 408 GAP IN PDB ENTRY  
 SEQADV 1GC1 G SWS P04578 GLU 409 GAP IN PDB ENTRY  
 SEQADV 1GC1 PRO G 470 SWS P04578 LEU 470 CONFLICT

SEQRES 1 G 321 GLY ALA ARG SER GLU VAL VAL LEU VAL ASN VAL THR GLU  
 SEQRES 2 G 321 ASN PHE ASN MET TRP LYS ASN ASP MET VAL GLU GLN MET  
 SEQRES 3 G 321 HIS GLU ASP ILE ILE SER LEU TRP ASP GLN SER LEU LYS  
 SEQRES 4 G 321 PRO CYS VAL LYS LEU THR PRO LEU CYS VAL GLY ALA GLY  
 SEQRES 5 G 321 SER CYS ASN THR SER VAL ILE THR GLN ALA CYS PRO LYS  
 SEQRES 6 G 321 VAL SER PHE GLU PRO ILE PRO ILE HIS TYR CYS ALA PRO  
 SEQRES 7 G 321 ALA GLY PHE ALA ILE LEU LYS CYS ASN ASN LYS THR PHE  
 SEQRES 8 G 321 ASN GLY THR GLY PRO CYS THR ASN VAL SER THR VAL GLN  
 SEQRES 9 G 321 CYS THR HIS GLY ILE ARG PRO VAL VAL SER THR GLN LEU  
 SEQRES 10 G 321 LEU LEU ASN GLY SER LEU ALA GLU GLU GLU VAL VAL ILE  
 SEQRES 11 G 321 ARG SER VAL ASN PHE THR ASP ASN ALA LYS THR ILE ILE  
 SEQRES 12 G 321 VAL GLN LEU ASN THR SER VAL GLU ILE ASN CYS THR GLY  
 SEQRES 13 G 321 ALA GLY HIS CYS ASN ILE SER ARG ALA LYS TRP ASN ASN  
 SEQRES 14 G 321 THR LEU LYS GLN ILE ALA SER LYS LEU ARG GLU GLN PHE  
 SEQRES 15 G 321 GLY ASN ASN LYS THR ILE ILE PHE LYS GLN SER SER GLY  
 SEQRES 16 G 321 GLY ASP PRO GLU ILE VAL THR HIS SER PHE ASN CYS GLY  
 SEQRES 17 G 321 GLY GLU PHE PHE TYR CYS ASN SER THR GLN LEU PHE ASN  
 SEQRES 18 G 321 SER THR TRP PHE ASN SER THR TRP SER THR LYS GLY SER  
 SEQRES 19 G 321 ASN ASN THR GLU GLY SER ASP THR ILE THR LEU PRO CYS  
 SEQRES 20 G 321 ARG ILE LYS GLN ILE ILE ASN MET TRP GLN LYS VAL GLY  
 SEQRES 21 G 321 LYS ALA MET TYR ALA PRO PRO ILE SER GLY GLN ILE ARG  
 SEQRES 22 G 321 CYS SER SER ASN ILE THR GLY LEU LEU LEU THR ARG ASP  
 SEQRES 23 G 321 GLY GLY ASN SER ASN ASN GLU SER GLU ILE PHE ARG PRO  
 SEQRES 24 G 321 GLY GLY GLY ASP MET ARG ASP ASN TRP ARG SER GLU LEU  
 SEQRES 25 G 321 TYR LYS TYR LYS VAL VAL LYS ILE GLU

SEQRES 1 C 185 LYS LYS VAL VAL LEU GLY LYS LYS GLY ASP THR VAL GLU  
 SEQRES 2 C 185 LEU THR CYS THR ALA SER GLN LYS LYS SER ILE GLN PHE  
 SEQRES 3 C 185 HIS TRP LYS ASN SER ASN GLN ILE LYS ILE LEU GLY ASN  
 SEQRES 4 C 185 GLN GLY SER PHE LEU THR LYS GLY PRO SER LYS LEU ASN  
 SEQRES 5 C 185 ASP ARG ALA ASP SER ARG ARG SER LEU TRP ASP GLN GLY  
 SEQRES 6 C 185 ASN PHE PRO LEU ILE ILE LYS ASN LEU LYS ILE GLU ASP  
 SEQRES 7 C 185 SER ASP THR TYR ILE CYS GLU VAL GLU ASP GLN LYS GLU  
 SEQRES 8 C 185 GLU VAL GLN LEU LEU VAL PHE GLY LEU THR ALA ASN SER  
 SEQRES 9 C 185 ASP THR HIS LEU LEU GLN GLY GLN SER LEU THR LEU THR  
 SEQRES 10 C 185 LEU GLU SER PRO PRO GLY SER SER PRO SER VAL GLN CYS  
 SEQRES 11 C 185 ARG SER PRO ARG GLY LYS ASN ILE GLN GLY GLY LYS THR  
 SEQRES 12 C 185 LEU SER VAL SER GLN LEU GLU LEU GLN ASP SER GLY THR  
 SEQRES 13 C 185 TRP THR CYS THR VAL LEU GLN ASN GLN LYS LYS VAL GLU  
 SEQRES 14 C 185 PHE LYS ILE ASP ILE VAL VAL LEU ALA PHE GLN LYS ALA  
 SEQRES 15 C 185 SER ASN THR

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FIG. 53-6

SEQRES 2 L 213 SER PRO GLY GLU ARG ALA THR LEU SER CYS ARG ALA SER  
 SEQRES 3 L 213 GLU SER VAL SER SER ASP LEU ALA TRP TYR GLN GLN LYS  
 SEQRES 4 L 213 PRO GLY GLN ALA PRO ARG LEU LEU ILE TYR GLY ALA SER  
 SEQRES 5 L 213 THR ARG ALA THR GLY VAL PRO ALA ARG PHE SER GLY SER  
 SEQRES 6 L 213 GLY SER GLY ALA GLU PHE THR LEU THR ILE SER SER LEU  
 SEQRES 7 L 213 GLN SER GLU ASP PHE ALA VAL TYR TYR CYS GLN GLN TYR  
 SEQRES 8 L 213 ASN ASN TRP PRO PRO ARG TYR THR PHE GLY GLN GLY THR  
 SEQRES 9 L 213 ARG LEU GLU ILE LYS ARG THR VAL ALA ALA PRO SER VAL  
 SEQRES 10 L 213 PHE ILE PHE PRO PRO SER ASP GLU GLN LEU LYS SER GLY  
 SEQRES 11 L 213 THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO  
 SEQRES 12 L 213 ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU  
 SEQRES 13 L 213 GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP  
 SEQRES 14 L 213 SER LYS ASP SER THR TYR SER LEU SER SER THR LEU THR  
 SEQRES 15 L 213 LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA  
 SEQRES 16 L 213 CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR  
 SEQRES 17 L 213 LYS SER PHE ASN ARG  
 SEQRES 1 H 229 GLN VAL GLN LEU LEU GLU SER GLY ALA GLU VAL LYS LYS  
 SEQRES 2 H 229 PRO GLY SER SER VAL LYS VAL SER CYS LYS ALA SER GLY  
 SEQRES 3 H 229 ASP THR PHE ILE ARG TYR SER PHE THR TRP VAL ARG GLN  
 SEQRES 4 H 229 ALA PRO GLY GLN GLY LEU GLU TRP MET GLY ARG ILE ILE  
 SEQRES 5 H 229 THR ILE LEU ASP VAL ALA HIS TYR ALA PRO HIS LEU GLN  
 SEQRES 6 H 229 GLY ARG VAL THR ILE THR ALA ASP LYS SER THR SER THR  
 SEQRES 7 H 229 VAL TYR LEU GLU LEU ARG ASN LEU ARG SER ASP ASP THR  
 SEQRES 8 H 229 ALA VAL TYR PHE CYS ALA GLY VAL TYR GLU GLY GLU ALA  
 SEQRES 9 H 229 ASP GLU GLY GLU TYR ASP ASN ASN GLY PHE LEU LYS HIS  
 SEQRES 10 H 229 TRP GLY GLN GLY THR LEU VAL THR VAL THR SER ALA SER  
 SEQRES 11 H 229 THR LYS GLY PRO SER VAL PHE PRO LEU ALA PRO SER SER  
 SEQRES 12 H 229 LYS SER THR SER GLY GLY THR ALA ALA LEU GLY CYS LEU  
 SEQRES 13 H 229 VAL LYS ASP TYR PHE PRO GLN PRO VAL THR VAL SER TRP  
 SEQRES 14 H 229 ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO  
 SEQRES 15 H 229 ALA VAL LEU GLN SER SER GLY LEU TYR SER LEU SER SER  
 SEQRES 16 H 229 VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR  
 SEQRES 17 H 229 TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS  
 SEQRES 18 H 229 VAL ASP LYS LYS VAL GLU PRO LYS  
 HET NAG G 697 14  
 HET NAG G 734 14  
 HET NAG G 762 14  
 HET NAG G 776 14  
 HET NAG G 789 14  
 HET NAG G 795 14  
 HET NAG G 832 14  
 HET NAG G 839 14  
 HET NAG G 886 14  
 HET NAG G 892 14  
 HET NAG G 948 14  
 HET FUC G 735 10  
 HET FUC G 796 10  
 HET FUC G 893 10  
 HET FUC G 949 10  
 HETNAM NAG N-ACETYL-D-GLUCOSAMINE  
 HETNAM FUC FUCOSE  
 FORMUL 5 NAG 11(C8 H15 N1 O6)  
 FORMUL 6 FUC 4(C6 H12 O5)  
 FORMUL 7 HOH \*603(H2 O1)  
 HELIX 1 GA1 MET G 100 LEU G 116 1 17  
 HELIX 2 GA2 ARG G 335 SER G 347 1 13  
 HELIX 3 GA3 ASP G 368 THR G 373 1 6  
 HELIX 4 GA4 THR G 388 PHE G 391 5 SLIGHTLY NON-STANDARD 4  
 HELIX 5 GA5 MET G 475 TYR G 484 1 10  
 HELIX 6 CA1 ARG C 58 GLY C 65 5 IRREGULAR 8  
 HELIX 7 CA2 LYS C 75 SER C 79 5 5  
 HELIX 8 CA3 GLU C 150 SER C 154 5 5  
 HELIX 9 LA1 SER L 123 GLY L 130 1 8  
 HELIX 10 LA2 LYS L 185 GLU L 189 1 5  
 HELIX 11 HA1 THR H 28 ILE H 30 5 3  
 HELIX 12 HA2 ARG H 87 THR H 91 5 5  
 HELIX 13 HA3 SER H 171 ALA H 173 5 3  
 SHEET 1 A 2 ASN G 92 ASN G 94 0  
 SHEET 2 A 2 GLY G 237 CYS G 239 -1  
 CRYST 1 R 4 SED G 100 H F G 201 0

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FIG. 53-7 SHEET 3 B4 VAL G 430 TYR G 435 -1  
 SHEET 4 B4 GLN G 422 MET G 426 -1  
 SHEET 1 C1 PRO G 214 ALA G 219 0  
 SHEET 2 C2 GLN G 246 ILE G 251 -1  
 SHEET 1 D3 ASN G 241 VAL G 245 0  
 SHEET 2 D3 GLY G 222 ASN G 229 -1  
 SHEET 3 D3 LYS G 485 ILE G 491 -1  
 SHEET 1 E7 LEU G 261 GLY G 263 0  
 SHEET 2 E7 ILE G 443 ILE G 449 1  
 SHEET 3 E7 VAL G 292 GLY G 298 -1  
 SHEET 4 E7 GLY G 329 SER G 334 -1  
 SHEET 5 E7 ASP G 412 LYS G 421 -1  
 SHEET 6 E7 GLU G 381 ASN G 386 -1  
 SHEET 7 E7 HIS G 374 CYS G 378 -1  
 SHEET 1 F6 VAL G 271 ARG G 273 0  
 SHEET 2 F6 ILE G 284 LEU G 288 -1  
 SHEET 3 F6 THR G 450 ASP G 457 -1  
 SHEET 4 F6 GLU G 464 GLY G 471 -1  
 SHEET 5 F6 THR G 358 LYS G 362 1  
 SHEET 6 F6 SER G 393 TRP G 395 -1  
 SHEET 1 G7 LYS C 2 LYS C 7 0  
 SHEET 2 G7 GLN C 89 PHE C 98 1 N GLN C 94 O LYS C 2  
 SHEET 3 G7 ASP C 80 VAL C 86 -1 N VAL C 86 O GLN C 89  
 SHEET 4 G7 HIS C 27 LYS C 29 -1 N LYS C 29 O ILE C 83  
 SHEET 5 G7 LYS C 35 GLN C 40 -1 N LEU C 37 O TRP C 28  
 SHEET 6 G7 PHE C 43 LYS C 46 -1 N THR C 45 O GLY C 38  
 SHEET 7 G7 GLY G 366 GLY G 367 -1 N GLY G 367 O LEU C 44  
 SHEET 1 H2 VAL C 12 LEU C 14 0  
 SHEET 2 H2 LEU C 69 ILE C 71 -1 N ILE C 71 O VAL C 12  
 SHEET 1 I3 GLY C 99 ALA C 102 0  
 SHEET 2 I3 LEU C 114 GLU C 119 -1 N GLU C 119 O GLY C 99  
 SHEET 3 I3 THR C 143 VAL C 146 -1 N VAL C 146 O LEU C 114  
 SHEET 1 J2 HIS C 107 LEU C 109 0  
 SHEET 2 J2 VAL C 175 LEU C 177 1 N VAL C 175 O LEU C 108  
 SHEET 1 K4 ASNC 137 GLY C 140 0  
 SHEET 2 K4 SER C 127 ARG C 131 -1 N CYS C 130 O ILE C 138  
 SHEET 3 K4 GLY C 155 GLN C 163 -1 N LEU C 162 O SER C 127  
 SHEET 4 K4 LYS C 166 ILE C 174 -1 N ILE C 174 O GLY C 155  
 SHEET 1 L4 LEU L 4 GLN L 6 0  
 SHEET 2 L4 ALA L 19 ALA L 25 -1 N ARG L 24 O THR L 5  
 SHEET 3 L4 GLU L 70 ILE L 75 -1 N ILE L 75 O ALA L 19  
 SHEET 4 L4 PHE L 62 SER L 67 -1 N SER L 67 O GLU L 70  
 SHEET 1 M5 THR L 10 VAL L 13 0  
 SHEET 2 M5 THR L 104 ILE L 108 1 N ARG L 105 O LEU L 11  
 SHEET 3 M5 ALA L 84 GLN L 90 -1 N TYR L 86 O THR L 104  
 SHEET 4 M5 LEU L 33 GLN L 38 -1 N GLN L 38 O VAL L 85  
 SHEET 5 M5 ARG L 45 ILE L 48 -1 N ILE L 48 O TRP L 35  
 SHEET 1 N4 SER L 116 PHE L 120 0  
 SHEET 2 N4 THR L 131 ASN L 139 -1 N ASN L 139 O SER L 116  
 SHEET 3 N4 LEU L 177 SER L 184 -1 N LEU L 183 O ALA L 132  
 SHEET 4 N4 SER L 161 VAL L 165 -1 N SER L 164 O SER L 178  
 SHEET 1 O3 LYS L 147 TRP L 150 0  
 SHEET 2 O3 VAL L 193 THR L 199 -1 N THR L 199 O LYS L 147  
 SHEET 3 O3 VAL L 207 ASN L 212 -1 N PHE L 211 O TYR L 194  
 SHEET 1 P4 GLN H 3 GLU H 6 0  
 SHEET 2 P4 VAL H 18 SER H 25 -1 N SER H 25 O GLN H 3  
 SHEET 3 P4 THR H 78 LEU H 83 -1 N LEU H 83 O VAL H 18  
 SHEET 4 P4 VAL H 68 ASP H 73 -1 N ASP H 73 O THR H 78  
 SHEET 1 Q6 GLU H 10 LYS H 12 0  
 SHEET 2 Q6 THR H 122 VAL H 126 1 N THR H 125 O GLU H 10  
 SHEET 3 Q6 ALA H 92 TYR H 100 -1 N TYR H 94 O THR H 122  
 SHEET 4 Q6 TYR H 32 GLN H 39 -1 N GLN H 39 O VAL H 93  
 SHEET 5 Q6 LEU H 45 ILE H 52 -1 N ILE H 51 O PHE H 34  
 SHEET 6 Q6 VAL H 57 TYR H 60 -1 N HIS H 59 O ARG H 50  
 SHEET 1 R4 SER H 135 LEU H 139 0  
 SHEET 2 R4 THR H 150 TYR H 160 -1 N LYS H 158 O SER H 135  
 SHEET 3 R4 TYR H 191 PRO H 200 -1 N VAL H 199 O ALA H 151  
 SHEET 4 R4 VAL H 178 THR H 180 -1 N HIS H 179 O VAL H 196  
 SHEET 1 S3 VAL H 165 TRP H 169 0  
 SHEET 2 S3 THR H 210 HIS H 215 -1 N ASN H 214 O THR H 166



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FIG. 53-8

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SSBOND 1 CYS G 119 CYS G 205
SSBOND 2 CYS G 126 CYS G 196
SSBOND 3 CYS G 218 CYS G 247
SSBOND 4 CYS G 228 CYS G 239
SSBOND 5 CYS G 296 CYS G 331
SSBOND 6 CYS G 378 CYS G 445
SSBOND 7 CYS G 385 CYS G 418
SSBOND 8 CYSC 16 CYSC 84
SSBOND 9 CYSC 130 CYSC 159
SSBOND 10 CYSL 23 CYSL 88
SSBOND 11 CYSL 136 CYSL 196
SSBOND 12 CYSH 22 CYSH 96
SSBOND 13 CYSH 155 CYSH 211
LINK C1 NAG G 697 ND2 ASN G 197
LINK C1 NAG G 734 ND2 ASN G 234
LINK O6 NAG G 734 C1 FUC G 735
LINK C1 NAG G 762 ND2 ASN G 262
LINK C1 NAG G 776 ND2 ASN G 276
LINK C1 NAG G 789 ND2 ASN G 289
LINK C1 NAG G 795 ND2 ASN G 295
LINK O6 NAG G 795 C1 FUC G 796
LINK C1 NAG G 832 ND2 ASN G 332
LINK C1 NAG G 839 ND2 ASN G 339
LINK C1 NAG G 886 ND2 ASN G 386
LINK C1 NAG G 892 ND2 ASN G 392
LINK O6 NAG G 892 C1 FUC G 893
LINK C1 NAG G 948 ND2 ASN G 448
LINK O6 NAG G 948 C1 FUC G 949
CISPEP 1 TRPL 94 PROL 95 0 -1.61
SITE 1 O 1 HOH 1000
CRYST1 71.640 88.130 196.700 90.00 90.00 90.00 P 2 2 21 4
ORIGX1 1.000000 0.000000 0.000000 0.000000
ORIGX2 0.000000 1.000000 0.000000 0.000000
ORIGX3 0.000000 0.000000 1.000000 0.000000
SCALE1 0.013959 0.000000 0.000000 0.000000
SCALE2 0.000000 0.011347 0.000000 0.000000
SCALE3 0.000000 0.000000 0.005084 0.000000
ATOM 1 N THR G 90 30.031 -50.064 78.936 1.00 42.55 N
ATOM 2 CA THR G 90 30.956 -49.288 79.751 1.00 43.59 C
ATOM 3 C THR G 90 32.160 -48.859 78.914 1.00 43.84 C
ATOM 4 O THR G 90 32.133 -48.983 77.690 1.00 43.64 O
ATOM 5 CB THR G 90 31.434 -50.091 80.976 1.00 43.87 C
ATOM 6 OG1 THR G 90 32.164 -49.231 81.860 1.00 44.69 O
ATOM 7 CG2 THR G 90 32.341 -51.244 80.546 1.00 44.10 C
ATOM 8 N GLU G 91 33.197 -48.347 79.579 1.00 44.15 N
ATOM 9 CA GLU G 91 34.411 -47.885 78.916 1.00 44.60 C
ATOM 10 C GLU G 91 34.013 -47.006 77.729 1.00 44.76 C
ATOM 11 O GLU G 91 34.031 -47.437 76.570 1.00 44.30 O
ATOM 12 CB GLU G 91 35.268 -49.083 78.488 1.00 45.29 C
ATOM 13 CG GLU G 91 36.609 -48.739 77.835 1.00 46.21 C
ATOM 14 CD GLU G 91 37.492 -47.838 78.686 1.00 46.69 C
ATOM 15 OE1 GLU G 91 37.408 -47.892 79.934 1.00 46.43 O
ATOM 16 OE2 GLU G 91 38.283 -47.074 78.097 1.00 46.96 O
ATOM 17 N ASN G 92 33.606 -45.779 78.038 1.00 45.37 N
ATOM 18 CA ASN G 92 33.158 -44.849 77.011 1.00 45.12 C
ATOM 19 C ASN G 92 33.960 -43.555 77.009 1.00 43.64 C
ATOM 20 O ASN G 92 34.841 -43.357 77.844 1.00 43.30 O
ATOM 21 CB ASN G 92 31.670 -44.551 77.193 1.00 46.34 C
ATOM 22 CG ASN G 92 30.946 -44.408 75.875 1.00 47.98 C
ATOM 23 OD1 ASN G 92 30.957 -43.340 75.264 1.00 50.80 O
ATOM 24 ND2 ASN G 92 30.327 -45.488 75.414 1.00 46.76 N
ATOM 25 N PHE G 93 33.643 -42.671 76.072 1.00 42.38 N
ATOM 26 CA PHE G 93 34.349 -41.405 75.954 1.00 41.75 C
ATOM 27 C PHE G 93 33.480 -40.164 76.196 1.00 40.40 C
ATOM 28 O PHE G 93 32.328 -40.096 75.745 1.00 39.86 O
ATOM 29 CB PHE G 93 35.022 -41.319 74.582 1.00 42.32 C
ATOM 30 CG PHE G 93 35.668 -39.999 74.316 1.00 44.10 C
ATOM 31 CD1 PHE G 93 36.893 -39.686 74.886 1.00 44.33 C
ATOM 32 CD2 PHE G 93 35.035 -39.055 73.513 1.00 44.30 C
ATOM 33 CE1 PHE G 93 37.180 -38.453 74.663 1.00 44.08 C

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FIG. 53-9

ATOM	35	CZ	PHE	G	93	36.837	-37.516	73.858	1.00	43.72	C
ATOM	36	N	ASN	G	94	34.077	-39.182	76.873	1.00	39.00	N
ATOM	37	CA	ASN	G	94	33.454	-37.897	77.210	1.00	37.42	C
ATOM	38	C	ASN	G	94	34.517	-36.797	77.002	1.00	37.03	C
ATOM	39	O	ASN	G	94	35.710	-37.108	76.896	1.00	36.49	O
ATOM	40	CB	ASN	G	94	33.002	-37.896	78.679	1.00	35.90	C
ATOM	41	CG	ASN	G	94	31.830	-38.834	78.945	1.00	34.52	C
ATOM	42	OD1	ASN	G	94	31.979	-40.057	78.952	1.00	33.54	O
ATOM	43	ND2	ASN	G	94	30.665	-38.261	79.205	1.00	34.56	N
ATOM	44	N	MET	G	95	34.107	-35.524	76.958	1.00	37.83	N
ATOM	45	CA	MET	G	95	35.065	-34.420	76.771	1.00	37.72	C
ATOM	46	C	MET	G	95	34.533	-32.980	76.950	1.00	37.31	C
ATOM	47	O	MET	G	95	33.358	-32.757	77.251	1.00	36.78	O
ATOM	48	CB	MET	G	95	35.718	-34.519	75.389	1.00	38.12	C
ATOM	49	CG	MET	G	95	34.916	-33.849	74.288	1.00	40.14	C
ATOM	50	SD	MET	G	95	35.944	-32.921	73.115	1.00	42.89	S
ATOM	51	CE	MET	G	95	37.369	-32.474	74.135	1.00	40.97	C
ATOM	52	N	TRP	G	96	35.426	-32.017	76.698	1.00	36.64	N
ATOM	53	CA	TRP	G	96	35.167	-30.571	76.769	1.00	34.44	C
ATOM	54	C	TRP	G	96	34.325	-30.111	75.579	1.00	32.91	C
ATOM	55	O	TRP	G	96	34.619	-29.091	74.957	1.00	31.85	O
ATOM	56	CB	TRP	G	96	36.504	-29.803	76.747	1.00	33.83	C
ATOM	57	CG	TRP	G	96	36.980	-29.352	78.091	1.00	33.15	C
ATOM	58	CD1	TRP	G	96	37.581	-30.109	79.045	1.00	33.76	C
ATOM	59	CD2	TRP	G	96	36.830	-28.044	78.652	1.00	34.00	C
ATOM	60	NE1	TRP	G	96	37.806	-29.360	80.175	1.00	35.56	N
ATOM	61	CE2	TRP	G	96	37.352	-28.087	79.960	1.00	34.55	C
ATOM	62	CE3	TRP	G	96	36.296	-26.836	78.177	1.00	32.92	C
ATOM	63	CZ2	TRP	G	96	37.355	-26.971	80.800	1.00	34.75	C
ATOM	64	CZ3	TRP	G	96	36.301	-25.733	79.008	1.00	32.95	C
ATOM	65	CH2	TRP	G	96	36.827	-25.806	80.307	1.00	33.90	C
ATOM	66	N	LYS	G	97	33.284	-30.874	75.270	1.00	33.26	N
ATOM	67	CA	LYS	G	97	32.403	-30.595	74.142	1.00	32.78	C
ATOM	68	C	LYS	G	97	31.005	-30.221	74.632	1.00	32.62	C
ATOM	69	O	LYS	G	97	30.731	-29.041	74.878	1.00	33.71	O
ATOM	70	CB	LYS	G	97	32.382	-31.812	73.189	1.00	32.07	C
ATOM	71	CG	LYS	G	97	31.271	-31.849	72.148	1.00	31.66	C
ATOM	72	CD	LYS	G	97	31.240	-30.621	71.251	1.00	31.98	C
ATOM	73	CE	LYS	G	97	32.430	-30.554	70.323	1.00	31.95	C
ATOM	74	NZ	LYS	G	97	32.231	-29.456	69.345	1.00	32.73	N
ATOM	75	N	ASN	G	98	30.137	-31.212	74.829	1.00	31.57	N
ATOM	76	CA	ASN	G	98	28.792	-30.901	75.276	1.00	32.25	C
ATOM	77	C	ASN	G	98	28.005	-32.017	75.980	1.00	32.40	C
ATOM	78	O	ASN	G	98	28.553	-32.777	76.776	1.00	31.37	O
ATOM	79	CB	ASN	G	98	27.987	-30.305	74.106	1.00	31.45	C
ATOM	80	CG	ASN	G	98	27.745	-31.296	72.972	1.00	31.55	C
ATOM	81	OD1	ASN	G	98	27.136	-30.945	71.961	1.00	30.95	O
ATOM	82	ND2	ASN	G	98	28.201	-32.535	73.137	1.00	31.27	N
ATOM	83	N	ASP	G	99	26.698	-31.999	75.737	1.00	33.77	N
ATOM	84	CA	ASP	G	99	25.677	-32.922	76.237	1.00	34.41	C
ATOM	85	C	ASP	G	99	24.477	-32.005	76.177	1.00	35.14	C
ATOM	86	O	ASP	G	99	23.555	-32.199	75.387	1.00	36.80	O
ATOM	87	CB	ASP	G	99	25.875	-33.361	77.690	1.00	32.72	C
ATOM	88	CG	ASP	G	99	24.658	-34.115	78.232	1.00	31.32	C
ATOM	89	OD1	ASP	G	99	24.205	-35.055	77.553	1.00	32.59	O
ATOM	90	OD2	ASP	G	99	24.127	-33.759	79.307	1.00	28.70	O
ATOM	91	N	MET	G	100	24.583	-30.919	76.929	1.00	35.52	N
ATOM	92	CA	MET	G	100	23.551	-29.907	76.990	1.00	35.08	C
ATOM	93	C	MET	G	100	24.197	-28.533	77.060	1.00	33.39	C
ATOM	94	O	MET	G	100	23.511	-27.557	77.314	1.00	33.51	O
ATOM	95	CB	MET	G	100	22.666	-30.103	78.227	1.00	38.36	C
ATOM	96	CG	MET	G	100	21.768	-31.322	78.195	1.00	40.24	C
ATOM	97	SD	MET	G	100	20.544	-31.193	76.890	1.00	41.93	S
ATOM	98	CE	MET	G	100	20.653	-32.816	76.172	1.00	39.92	C
ATOM	99	N	VAL	G	101	25.511	-28.441	76.860	1.00	31.09	N
ATOM	100	CA	VAL	G	101	26.157	-27.131	76.921	1.00	27.99	C
ATOM	101	C	VAL	G	101	25.490	-26.185	75.910	1.00	26.63	C
ATOM	102	O	VAL	G	101	24.965	-25.138	76.295	1.00	27.19	O
ATOM	103	CB	VAL	G	101	27.684	-27.211	76.701	1.00	26.80	C
ATOM	104	CG	VAL	G	101	28.314	-25.933	76.875	1.00	23.64	C

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FIG. 53-10

ATOM	106	N	GLU G 102	25.453 -26.572 74.639 1.00 23.53	N
ATOM	107	CA	GLU G 102	24.805 -25.744 73.629 1.00 21.32	C
ATOM	108	C	GLU G 102	23.298 -25.708 73.838 1.00 20.85	C
ATOM	109	O	GLU G 102	22.665 -24.674 73.615 1.00 23.56	O
ATOM	110	CB	GLU G 102	25.114 -26.253 72.225 1.00 20.82	C
ATOM	111	CG	GLU G 102	26.375 -25.686 71.605 1.00 18.31	C
ATOM	112	CD	GLU G 102	27.622 -25.948 72.431 1.00 16.74	C
ATOM	113	OE1	GLU G 102	27.821 -27.107 72.870 1.00 14.69	O
ATOM	114	OE2	GLU G 102	28.403 -24.988 72.635 1.00 14.10	O
ATOM	115	N	GLN G 103	22.726 -26.841 74.250 1.00 18.06	N
ATOM	116	CA	GLN G 103	21.283 -26.971 74.499 1.00 16.18	C
ATOM	117	C	GLN G 103	20.860 -26.063 75.645 1.00 14.68	C
ATOM	118	O	GLN G 103	20.054 -25.155 75.461 1.00 16.26	O
ATOM	119	CB	GLN G 103	20.933 -28.419 74.859 1.00 17.03	C
ATOM	120	CG	GLN G 103	19.845 -29.041 74.004 1.00 16.72	C
ATOM	121	CD	GLN G 103	18.527 -28.346 74.159 1.00 17.00	C
ATOM	122	OE1	GLN G 103	18.001 -27.767 73.209 1.00 16.51	O
ATOM	123	NE2	GLN G 103	17.961 -28.425 75.352 1.00 19.08	N
ATOM	124	N	MET G 104	21.383 -26.352 76.832 1.00 11.83	N
ATOM	125	CA	MET G 104	21.128 -25.583 78.043 1.00 11.35	C
ATOM	126	C	MET G 104	21.302 -24.091 77.761 1.00 11.72	C
ATOM	127	O	MET G 104	20.382 -23.305 77.997 1.00 10.83	O
ATOM	128	CB	MET G 104	22.121 -26.001 79.120 1.00 11.71	C
ATOM	129	CG	MET G 104	21.764 -25.618 80.530 1.00 11.54	C
ATOM	130	SD	MET G 104	23.083 -26.186 81.587 1.00 11.76	S
ATOM	131	CE	MET G 104	22.640 -25.382 83.126 1.00 13.15	C
ATOM	132	N	HIS G 105	22.463 -23.711 77.220 1.00 11.06	N
ATOM	133	CA	HIS G 105	22.746 -22.314 76.893 1.00 11.77	C
ATOM	134	C	HIS G 105	21.541 -21.681 76.196 1.00 13.11	C
ATOM	135	O	HIS G 105	21.053 -20.637 76.625 1.00 12.48	O
ATOM	136	CB	HIS G 105	23.995 -22.199 76.008 1.00 10.23	C
ATOM	137	CG	HIS G 105	24.614 -20.839 76.003 1.00 8.87	C
ATOM	138	ND1	HIS G 105	24.918 -20.177 77.167 1.00 7.75	N
ATOM	139	CD2	HIS G 105	25.039 -20.085 74.950 1.00 10.05	C
ATOM	140	CE1	HIS G 105	25.513 -19.058 76.810 1.00 9.56	C
ATOM	141	NE2	HIS G 105	25.611 -18.954 75.475 1.00 7.33	N
ATOM	142	N	GLU G 106	20.998 -22.370 75.194 1.00 15.32	N
ATOM	143	CA	GLU G 106	19.843 -21.862 74.469 1.00 17.17	C
ATOM	144	C	GLU G 106	18.564 -21.908 75.293 1.00 17.51	C
ATOM	145	O	GLU G 106	17.652 -21.115 75.060 1.00 19.56	O
ATOM	146	CB	GLU G 106	19.663 -22.586 73.132 1.00 20.59	C
ATOM	147	CG	GLU G 106	20.773 -22.299 72.104 1.00 28.21	C
ATOM	148	CD	GLU G 106	20.999 -20.802 71.832 1.00 32.28	C
ATOM	149	OE1	GLU G 106	20.005 -20.050 71.719 1.00 34.24	O
ATOM	150	OE2	GLU G 106	22.179 -20.386 71.723 1.00 31.84	O
ATOM	151	N	ASP G 107	18.477 -22.823 76.254 1.00 17.54	N
ATOM	152	CA	ASP G 107	17.283 -22.881 77.101 1.00 17.03	C
ATOM	153	C	ASP G 107	17.315 -21.697 78.059 1.00 14.26	C
ATOM	154	O	ASP G 107	16.332 -20.973 78.207 1.00 11.84	O
ATOM	155	CB	ASP G 107	17.225 -24.182 77.899 1.00 21.39	C
ATOM	156	CG	ASP G 107	16.535 -25.310 77.140 1.00 26.46	C
ATOM	157	OD1	ASP G 107	15.279 -25.348 77.098 1.00 28.30	O
ATOM	158	OD2	ASP G 107	17.254 -26.195 76.628 1.00 28.96	O
ATOM	159	N	ILE G 108	18.478 -21.486 78.674 1.00 13.84	N
ATOM	160	CA	ILE G 108	18.711 -20.388 79.615 1.00 12.27	C
ATOM	161	C	ILE G 108	18.596 -19.027 78.928 1.00 12.24	C
ATOM	162	O	ILE G 108	17.996 -18.103 79.477 1.00 14.39	O
ATOM	163	CB	ILE G 108	20.074 -20.519 80.303 1.00 10.08	C
ATOM	164	CG1	ILE G 108	20.227 -21.943 80.871 1.00 9.55	C
ATOM	165	CG2	ILE G 108	20.191 -19.495 81.422 1.00 8.16	C
ATOM	166	CD1	ILE G 108	19.022 -22.441 81.680 1.00 2.00	C
ATOM	167	N	ILE G 109	19.139 -18.897 77.723 1.00 9.86	N
ATOM	168	CA	ILE G 109	19.004 -17.640 77.006 1.00 8.89	C
ATOM	169	C	ILE G 109	17.518 -17.407 76.764 1.00 7.93	C
ATOM	170	O	ILE G 109	17.022 -16.303 76.938 1.00 9.04	O
ATOM	171	CB	ILE G 109	19.745 -17.633 75.642 1.00 7.59	C
ATOM	172	CG1	ILE G 109	21.255 -17.655 75.854 1.00 5.11	C
ATOM	173	CG2	ILE G 109	19.413 -16.368 74.874 1.00 9.22	C
ATOM	174	CD1	ILE G 109	22.033 -17.460 74.588 1.00 3.72	C
ATOM	175	N	SER G 110	16.701 -18.463 76.436 1.00 7.80	N

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FIG. 53-11

ATOM 177	C	SER G 110	14.530	-18.251	77.454	1.00	11.75	C
ATOM 178	O	SER G 110	13.324	-17.967	77.425	1.00	11.41	O
ATOM 179	CB	SER G 110	14.886	-19.477	75.283	1.00	9.57	C
ATOM 180	OG	SER G 110	15.657	-19.524	74.088	1.00	8.93	O
ATOM 181	N	LEU G 111	15.174	-18.511	78.584	1.00	13.81	N
ATOM 182	CA	LEU G 111	14.495	-18.467	79.867	1.00	14.15	C
ATOM 183	C	LEU G 111	14.586	-17.035	80.380	1.00	15.33	C
ATOM 184	O	LEU G 111	13.588	-16.428	80.786	1.00	14.92	O
ATOM 185	CB	LEU G 111	15.159	-19.445	80.831	1.00	13.12	C
ATOM 186	CG	LEU G 111	14.248	-19.938	81.949	1.00	14.99	C
ATOM 187	CD1	LEU G 111	14.601	-21.370	82.306	1.00	16.86	C
ATOM 188	CD2	LEU G 111	14.349	-19.008	83.150	1.00	14.95	C
ATOM 189	N	TRP G 112	15.785	-16.476	80.286	1.00	16.51	N
ATOM 190	CA	TRP G 112	16.031	-15.113	80.715	1.00	17.45	C
ATOM 191	C	TRP G 112	15.124	-14.162	79.974	1.00	18.63	C
ATOM 192	O	TRP G 112	14.487	-13.314	80.592	1.00	21.62	O
ATOM 193	CB	TRP G 112	17.481	-14.741	80.465	1.00	16.89	C
ATOM 194	CG	TRP G 112	18.347	-15.026	81.623	1.00	15.36	C
ATOM 195	CD1	TRP G 112	18.492	-16.216	82.278	1.00	13.64	C
ATOM 196	CD2	TRP G 112	19.175	-14.086	82.302	1.00	14.57	C
ATOM 197	NE1	TRP G 112	19.360	-16.068	83.331	1.00	14.50	N
ATOM 198	CE2	TRP G 112	19.793	-14.769	83.369	1.00	14.49	C
ATOM 199	CE3	TRP G 112	19.453	-12.728	82.113	1.00	11.21	C
ATOM 200	CZ2	TRP G 112	20.675	-14.137	84.245	1.00	13.94	C
ATOM 201	CZ3	TRP G 112	20.324	-12.103	82.979	1.00	11.75	C
ATOM 202	CH2	TRP G 112	20.926	-12.804	84.033	1.00	13.78	C
ATOM 203	N	ASP G 113	15.051	-14.323	78.658	1.00	18.33	N
ATOM 204	CA	ASP G 113	14.208	-13.490	77.818	1.00	19.69	C
ATOM 205	C	ASP G 113	12.776	-13.400	78.354	1.00	21.06	C
ATOM 206	O	ASP G 113	12.250	-12.302	78.544	1.00	21.21	O
ATOM 207	CB	ASP G 113	14.200	-14.022	76.377	1.00	19.57	C
ATOM 208	CG	ASP G 113	15.518	-13.767	75.633	1.00	19.88	C
ATOM 209	OD1	ASP G 113	16.541	-13.418	76.267	1.00	18.64	O
ATOM 210	OD2	ASP G 113	15.527	-13.928	74.391	1.00	19.87	O
ATOM 211	N	GLN G 114	12.156	-14.553	78.618	1.00	23.29	N
ATOM 212	CA	GLN G 114	10.776	-14.604	79.131	1.00	24.16	C
ATOM 213	C	GLN G 114	10.638	-14.027	80.545	1.00	24.98	C
ATOM 214	O	GLN G 114	9.553	-13.601	80.946	1.00	25.23	O
ATOM 215	CB	GLN G 114	10.228	-16.048	79.117	1.00	23.58	C
ATOM 216	CG	GLN G 114	10.735	-16.953	80.263	1.00	23.77	C
ATOM 217	CD	GLN G 114	10.087	-18.346	80.303	1.00	21.80	C
ATOM 218	OE1	GLN G 114	9.657	-18.810	81.357	1.00	20.50	O
ATOM 219	NE2	GLN G 114	10.071	-19.030	79.172	1.00	20.83	N
ATOM 220	N	SER G 115	11.739	-13.989	81.286	1.00	26.32	N
ATOM 221	CA	SER G 115	11.724	-13.482	82.649	1.00	28.15	C
ATOM 222	C	SER G 115	12.191	-12.033	82.789	1.00	27.92	C
ATOM 223	O	SER G 115	11.367	-11.109	82.795	1.00	29.96	O
ATOM 224	CB	SER G 115	12.549	-14.409	83.547	1.00	31.07	C
ATOM 225	OG	SER G 115	12.333	-14.132	84.920	1.00	35.36	O
ATOM 226	N	LEU G 116	13.506	-11.829	82.870	1.00	26.47	N
ATOM 227	CA	LEU G 116	14.096	-10.494	83.041	1.00	24.17	C
ATOM 228	C	LEU G 116	14.051	-9.630	81.788	1.00	23.78	C
ATOM 229	O	LEU G 116	15.038	-9.517	81.068	1.00	24.42	O
ATOM 230	CB	LEU G 116	15.546	-10.616	83.522	1.00	22.24	C
ATOM 231	CG	LEU G 116	15.833	-11.024	84.969	1.00	19.18	C
ATOM 232	CD1	LEU G 116	17.241	-11.555	85.085	1.00	17.42	C
ATOM 233	CD2	LEU G 116	15.634	-9.831	85.893	1.00	20.14	C
ATOM 234	N	LYS G 117	12.902	-9.017	81.536	1.00	24.32	N
ATOM 235	CA	LYS G 117	12.727	-8.150	80.372	1.00	24.12	C
ATOM 236	C	LYS G 117	13.301	-6.739	80.575	1.00	24.20	C
ATOM 237	O	LYS G 117	13.048	-6.083	81.591	1.00	22.60	O
ATOM 238	CB	LYS G 117	11.248	-8.078	79.975	1.00	23.53	C
ATOM 239	CG	LYS G 117	10.791	-9.215	79.061	1.00	24.11	C
ATOM 240	CD	LYS G 117	9.275	-9.287	78.933	1.00	22.89	C
ATOM 241	CE	LYS G 117	8.693	-10.447	79.750	1.00	22.26	C
ATOM 242	NZ	LYS G 117	8.938	-10.378	81.232	1.00	21.42	N
ATOM 243	N	PRO G 118	14.136	-6.282	79.630	1.00	24.87	N
ATOM 244	CA	PRO G 118	14.745	-4.957	79.708	1.00	26.24	C
ATOM 245	C	PRO G 118	14.215	-4.016	78.632	1.00	28.46	C
ATOM 246	O	PRO G 118	13.010	-3.018	78.371	1.00	27.89	O

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FIG. 53-12	ATOM 248	CG	PRO G 118	16.058	-6.227	78.276	1.00	24.79	C
	ATOM 249	CD	PRO G 118	14.907	-7.134	78.705	1.00	25.85	C
	ATOM 250	N	CYS G 119	15.166	-3.317	78.023	1.00	30.90	N
	ATOM 251	CA	CYS G 119	14.951	-2.361	76.955	1.00	32.05	C
	ATOM 252	C	CYS G 119	16.293	-2.538	76.185	1.00	30.56	C
	ATOM 253	O	CYS G 119	17.284	-1.848	76.424	1.00	30.87	O
	ATOM 254	CB	CYS G 119	14.726	-0.972	77.587	1.00	33.32	C
	ATOM 255	SG	CYS G 119	13.194	-0.851	78.612	1.00	39.28	S
	ATOM 256	N	VAL G 120	16.312	-3.605	75.382	1.00	29.90	N
	ATOM 257	CA	VAL G 120	17.451	-4.101	74.585	1.00	27.91	C
	ATOM 258	C	VAL G 120	18.028	-3.209	73.489	1.00	27.39	C
	ATOM 259	O	VAL G 120	17.368	-2.310	73.002	1.00	29.19	O
	ATOM 260	CB	VAL G 120	17.082	-5.472	73.916	1.00	26.78	C
	ATOM 261	CG1	VAL G 120	18.324	-6.242	73.535	1.00	26.16	C
	ATOM 262	CG2	VAL G 120	16.206	-6.312	74.826	1.00	25.20	C
	ATOM 263	N	LYS G 121	19.251	-3.515	73.073	1.00	27.48	N
	ATOM 264	CA	LYS G 121	19.934	-2.790	72.011	1.00	28.16	C
	ATOM 265	C	LYS G 121	21.093	-3.658	71.491	1.00	28.51	C
	ATOM 266	O	LYS G 121	22.133	-3.779	72.143	1.00	27.76	O
	ATOM 267	CB	LYS G 121	20.450	-1.448	72.536	1.00	28.76	C
	ATOM 268	CG	LYS G 121	20.477	-0.360	71.480	1.00	28.67	C
	ATOM 269	CD	LYS G 121	20.967	0.952	72.030	1.00	29.16	C
	ATOM 270	CE	LYS G 121	22.438	0.889	72.369	1.00	29.64	C
	ATOM 271	NZ	LYS G 121	23.025	2.251	72.244	1.00	32.93	N
	ATOM 272	N	LEU G 122	20.890	-4.280	70.332	1.00	29.13	N
	ATOM 273	CA	LEU G 122	21.882	-5.169	69.721	1.00	29.85	C
	ATOM 274	C	LEU G 122	22.306	-4.696	68.330	1.00	31.68	C
	ATOM 275	O	LEU G 122	21.480	-4.206	67.557	1.00	30.70	O
	ATOM 276	CB	LEU G 122	21.333	-6.598	69.631	1.00	29.20	C
	ATOM 277	CG	LEU G 122	19.973	-6.806	68.952	1.00	29.73	C
	ATOM 278	CD1	LEU G 122	19.854	-8.232	68.431	1.00	29.60	C
	ATOM 279	CD2	LEU G 122	18.832	-6.471	69.903	1.00	28.04	C
	ATOM 280	N	THR G 123	23.573	-4.922	67.988	1.00	35.02	N
	ATOM 281	CA	THR G 123	24.128	-4.486	66.708	1.00	39.27	C
	ATOM 282	C	THR G 123	24.276	-5.430	65.517	1.00	43.14	C
	ATOM 283	O	THR G 123	25.073	-6.368	65.563	1.00	45.11	O
	ATOM 284	CB	THR G 123	25.533	-3.877	66.890	1.00	39.33	C
	ATOM 285	OG1	THR G 123	26.257	-4.621	67.883	1.00	37.86	O
	ATOM 286	CG2	THR G 123	25.451	-2.402	67.271	1.00	40.77	C
	ATOM 287	N	PRO G 124	23.466	-5.240	64.468	1.00	45.88	N
	ATOM 288	CA	PRO G 124	23.513	-6.047	63.242	1.00	47.10	C
	ATOM 289	C	PRO G 124	24.355	-5.185	62.292	1.00	47.86	C
	ATOM 290	O	PRO G 124	24.015	-4.029	62.048	1.00	46.46	O
	ATOM 291	CB	PRO G 124	22.051	-6.114	62.814	1.00	47.28	C
	ATOM 292	CG	PRO G 124	21.510	-4.836	63.265	1.00	47.43	C
	ATOM 293	CD	PRO G 124	22.137	-4.620	64.617	1.00	46.92	C
	ATOM 294	N	LEU G 125	25.461	-5.713	61.786	1.00	50.15	N
	ATOM 295	CA	LEU G 125	26.324	-4.890	60.946	1.00	53.58	C
	ATOM 296	C	LEU G 125	26.012	-4.529	59.498	1.00	55.92	C
	ATOM 297	O	LEU G 125	25.466	-5.314	58.719	1.00	55.97	O
	ATOM 298	CB	LEU G 125	27.797	-5.259	61.136	1.00	53.97	C
	ATOM 299	CG	LEU G 125	28.463	-4.311	62.143	1.00	54.12	C
	ATOM 300	CD1	LEU G 125	28.818	-2.975	61.498	1.00	54.49	C
	ATOM 301	CD2	LEU G 125	27.536	-4.081	63.328	1.00	54.73	C
	ATOM 302	N	CYS G 126	26.422	-3.305	59.178	1.00	58.50	N
	ATOM 303	CA	CYS G 126	26.244	-2.634	57.896	1.00	60.18	C
	ATOM 304	C	CYS G 126	26.585	-3.269	56.557	1.00	59.83	C
	ATOM 305	O	CYS G 126	27.185	-4.339	56.458	1.00	59.92	O
	ATOM 306	CB	CYS G 126	26.951	-1.283	57.945	1.00	61.77	C
	ATOM 307	SG	CYS G 126	26.277	-0.089	59.134	1.00	67.19	S
	ATOM 308	N	VAL G 127	26.206	-2.517	55.529	1.00	58.73	N
	ATOM 309	CA	VAL G 127	26.432	-2.814	54.121	1.00	58.05	C
	ATOM 310	C	VAL G 127	26.789	-1.430	53.582	1.00	57.40	C
	ATOM 311	O	VAL G 127	27.888	-1.211	53.066	1.00	57.78	O
	ATOM 312	CB	VAL G 127	25.145	-3.310	53.416	1.00	58.63	C
	ATOM 313	CG1	VAL G 127	25.332	-3.307	51.906	1.00	58.31	C
	ATOM 314	CG2	VAL G 127	24.796	-4.709	53.886	1.00	59.78	C
	ATOM 315	N	GLY G 128	25.869	-0.485	53.773	1.00	56.22	N
	ATOM 316	CA	GLY G 128	26.095	0.879	53.330	1.00	54.59	C
	ATOM 317	C	GLY G 128	24.880	1.554	52.717	1.00	53.61	C

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FIG. 53-13

ATOM	319	N	ALA	G	129	25.136	2.639	51.991	1.00	53.86	N
ATOM	320	CA	ALA	G	129	24.107	3.419	51.295	1.00	53.81	C
ATOM	321	C	ALA	G	129	22.957	3.928	52.169	1.00	53.84	C
ATOM	322	O	ALA	G	129	21.794	3.882	51.771	1.00	53.00	O
ATOM	323	CB	ALA	G	129	23.564	2.630	50.092	1.00	53.14	C
ATOM	324	N	GLY	G	194	23.291	4.435	53.351	1.00	54.62	N
ATOM	325	CA	GLY	G	194	22.276	4.956	54.251	1.00	55.99	C
ATOM	326	C	GLY	G	194	21.534	3.878	55.019	1.00	57.37	C
ATOM	327	O	GLY	G	194	20.858	4.169	56.013	1.00	57.33	O
ATOM	328	N	SER	G	195	21.665	2.634	54.566	1.00	58.65	N
ATOM	329	CA	SER	G	195	21.018	1.492	55.195	1.00	59.28	C
ATOM	330	C	SER	G	195	21.997	0.855	56.181	1.00	59.27	C
ATOM	331	O	SER	G	195	23.039	0.321	55.791	1.00	58.61	O
ATOM	332	CB	SER	G	195	20.605	0.477	54.122	1.00	59.90	C
ATOM	333	OG	SER	G	195	19.683	-0.475	54.626	1.00	61.03	O
ATOM	334	N	CYS	G	196	21.662	0.936	57.463	1.00	59.98	N
ATOM	335	CA	CYS	G	196	22.490	0.377	58.527	1.00	60.78	C
ATOM	336	C	CYS	G	196	21.642	0.079	59.756	1.00	59.75	C
ATOM	337	O	CYS	G	196	21.122	0.990	60.400	1.00	60.30	O
ATOM	338	CB	CYS	G	196	23.612	1.348	58.906	1.00	62.88	C
ATOM	339	SG	CYS	G	196	25.173	1.175	57.983	1.00	66.93	S
ATOM	340	N	ASN	G	197	21.472	-1.200	60.059	1.00	57.89	N
ATOM	341	CA	ASN	G	197	20.680	-1.593	61.212	1.00	55.54	C
ATOM	342	C	ASN	G	197	21.464	-1.640	62.523	1.00	52.35	C
ATOM	343	O	ASN	G	197	22.690	-1.738	62.534	1.00	51.55	O
ATOM	344	CB	ASN	G	197	19.912	-2.921	60.968	1.00	58.11	C
ATOM	345	CG	ASN	G	197	20.757	-4.005	60.276	1.00	59.71	C
ATOM	346	OD1	ASN	G	197	21.810	-3.721	59.710	1.00	62.77	O
ATOM	347	ND2	ASN	G	197	20.263	-5.243	60.269	1.00	60.06	N
ATOM	348	N	THR	G	198	20.724	-1.454	63.609	1.00	48.87	N
ATOM	349	CA	THR	G	198	21.197	-1.495	64.995	1.00	44.56	C
ATOM	350	C	THR	G	198	19.882	-1.452	65.755	1.00	41.54	C
ATOM	351	O	THR	G	198	19.346	-0.384	66.035	1.00	42.10	O
ATOM	352	CB	THR	G	198	22.085	-0.293	65.393	1.00	43.77	C
ATOM	353	OG1	THR	G	198	23.364	-0.405	64.755	1.00	43.48	O
ATOM	354	CG2	THR	G	198	22.302	-0.283	66.909	1.00	42.07	C
ATOM	355	N	SER	G	199	19.327	-2.632	65.986	1.00	37.87	N
ATOM	356	CA	SER	G	199	18.039	-2.778	66.642	1.00	35.19	C
ATOM	357	C	SER	G	199	17.930	-2.385	68.103	1.00	32.73	C
ATOM	358	O	SER	G	199	18.608	-2.957	68.963	1.00	32.29	O
ATOM	359	CB	SER	G	199	17.544	-4.213	66.472	1.00	36.29	C
ATOM	360	OG	SER	G	199	18.538	-5.150	66.853	1.00	37.38	O
ATOM	361	N	VAL	G	200	17.065	-1.409	68.374	1.00	29.80	N
ATOM	362	CA	VAL	G	200	16.804	-0.964	69.740	1.00	26.54	C
ATOM	363	C	VAL	G	200	15.398	-1.463	70.022	1.00	24.38	C
ATOM	364	O	VAL	G	200	14.560	-1.492	69.119	1.00	24.85	O
ATOM	365	CB	VAL	G	200	16.850	0.583	69.897	1.00	25.48	C
ATOM	366	CG1	VAL	G	200	18.070	1.152	69.184	1.00	24.83	C
ATOM	367	CG2	VAL	G	200	15.574	1.221	69.389	1.00	25.79	C
ATOM	368	N	ILE	G	201	15.156	-1.927	71.238	1.00	22.71	N
ATOM	369	CA	ILE	G	201	13.832	-2.423	71.601	1.00	21.84	C
ATOM	370	C	ILE	G	201	13.424	-1.849	72.944	1.00	21.54	C
ATOM	371	O	ILE	G	201	14.127	-1.993	73.942	1.00	21.04	O
ATOM	372	CB	ILE	G	201	13.757	-3.973	71.635	1.00	20.77	C
ATOM	373	CG1	ILE	G	201	13.888	-4.537	70.215	1.00	20.78	C
ATOM	374	CG2	ILE	G	201	12.436	-4.419	72.236	1.00	20.16	C
ATOM	375	CD1	ILE	G	201	13.760	-6.045	70.129	1.00	23.33	C
ATOM	376	N	THR	G	202	12.283	-1.179	72.941	1.00	21.75	N
ATOM	377	CA	THR	G	202	11.742	-0.550	74.125	1.00	22.67	C
ATOM	378	C	THR	G	202	10.596	-1.391	74.662	1.00	24.65	C
ATOM	379	O	THR	G	202	9.459	-1.285	74.205	1.00	25.31	O
ATOM	380	CB	THR	G	202	11.241	0.872	73.791	1.00	21.11	C
ATOM	381	OG1	THR	G	202	12.295	1.609	73.158	1.00	20.05	O
ATOM	382	CG2	THR	G	202	10.803	1.602	75.053	1.00	19.42	C
ATOM	383	N	GLN	G	203	10.909	-2.278	75.591	1.00	27.54	N
ATOM	384	CA	GLN	G	203	9.888	-3.133	76.180	1.00	30.82	C
ATOM	385	C	GLN	G	203	9.499	-2.468	77.471	1.00	33.16	C
ATOM	386	O	GLN	G	203	10.235	-1.623	77.986	1.00	32.53	O
ATOM	387	CB	GLN	G	203	10.448	-4.509	76.539	1.00	31.40	C
ATOM	388	CG	GLN	G	203	11.107	-5.770	75.477	1.00	32.25	C

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FIG. 53-14	ATOM	390	OE1 GLN G 203	12.826	-6.912	75.187	1.00	35.60	O
	ATOM	391	NE2 GLN G 203	12.212	-6.383	77.270	1.00	32.67	N
	ATOM	392	N ALA G 204	8.351	-2.866	78.007	1.00	36.76	N
	ATOM	393	CA ALA G 204	7.892	-2.330	79.273	1.00	40.59	C
	ATOM	394	C ALA G 204	8.815	-2.971	80.301	1.00	42.64	C
	ATOM	395	O ALA G 204	8.514	-4.047	80.819	1.00	43.43	O
	ATOM	396	CB ALA G 204	6.447	-2.728	79.527	1.00	40.97	C
	ATOM	397	N CYS G 205	9.999	-2.378	80.451	1.00	44.24	N
	ATOM	398	CA CYS G 205	11.030	-2.820	81.385	1.00	44.23	C
	ATOM	399	C CYS G 205	10.325	-3.002	82.743	1.00	44.07	C
	ATOM	400	O CYS G 205	9.854	-2.030	83.328	1.00	45.34	O
	ATOM	401	CB CYS G 205	12.133	-1.732	81.451	1.00	43.58	C
	ATOM	402	SG CYS G 205	13.597	-1.867	80.335	1.00	46.40	S
	ATOM	403	N PRO G 206	10.144	-4.260	83.202	1.00	43.68	N
	ATOM	404	CA PRO G 206	9.472	-4.532	84.480	1.00	42.68	C
	ATOM	405	C PRO G 206	10.306	-5.049	85.652	1.00	41.36	C
	ATOM	406	O PRO G 206	11.231	-5.851	85.477	1.00	40.87	O
	ATOM	407	CB PRO G 206	8.440	-5.567	84.079	1.00	43.26	C
	ATOM	408	CG PRO G 206	9.210	-6.423	83.081	1.00	44.31	C
	ATOM	409	CD PRO G 206	10.229	-5.495	82.401	1.00	44.01	C
	ATOM	410	N LYS G 207	9.914	-4.643	86.860	1.00	40.18	N
	ATOM	411	CA LYS G 207	10.598	-5.057	88.083	1.00	39.24	C
	ATOM	412	C LYS G 207	10.112	-6.419	88.558	1.00	40.55	C
	ATOM	413	O LYS G 207	9.253	-6.513	89.436	1.00	41.20	O
	ATOM	414	CB LYS G 207	10.412	-4.028	89.213	1.00	35.60	C
	ATOM	415	CG LYS G 207	11.073	-2.676	88.978	1.00	28.24	C
	ATOM	416	CD LYS G 207	12.523	-2.811	88.527	1.00	20.45	C
	ATOM	417	CE LYS G 207	13.447	-3.269	89.619	1.00	14.36	C
	ATOM	418	NZ LYS G 207	14.818	-3.500	89.066	1.00	12.04	N
	ATOM	419	N VAL G 208	10.652	-7.471	87.958	1.00	40.92	N
	ATOM	420	CA VAL G 208	10.283	-8.825	88.326	1.00	41.10	C
	ATOM	421	C VAL G 208	11.416	-9.383	89.178	1.00	42.22	C
	ATOM	422	O VAL G 208	12.452	-8.733	89.345	1.00	41.88	O
	ATOM	423	CB VAL G 208	10.086	-9.703	87.064	1.00	40.88	C
	ATOM	424	CG1 VAL G 208	11.435	-10.083	86.454	1.00	40.92	C
	ATOM	425	CG2 VAL G 208	9.255	-10.936	87.392	1.00	40.95	C
	ATOM	426	N SER G 209	11.211	-10.583	89.708	1.00	42.81	N
	ATOM	427	CA SER G 209	12.193	-11.271	90.534	1.00	42.90	C
	ATOM	428	C SER G 209	12.614	-12.559	89.826	1.00	43.05	C
	ATOM	429	O SER G 209	11.790	-13.447	89.576	1.00	43.93	O
	ATOM	430	CB SER G 209	11.560	-11.593	91.887	1.00	44.08	C
	ATOM	431	OG SER G 209	10.172	-11.851	91.723	1.00	44.85	O
	ATOM	432	N PHE G 210	13.887	-12.645	89.464	1.00	42.58	N
	ATOM	433	CA PHE G 210	14.395	-13.825	88.774	1.00	41.96	C
	ATOM	434	C PHE G 210	14.800	-14.899	89.784	1.00	41.92	C
	ATOM	435	O PHE G 210	15.612	-14.645	90.669	1.00	42.16	O
	ATOM	436	CB PHE G 210	15.582	-13.440	87.887	1.00	40.06	C
	ATOM	437	CG PHE G 210	16.117	-14.572	87.061	1.00	39.61	C
	ATOM	438	CD1 PHE G 210	15.277	-15.299	86.225	1.00	39.31	C
	ATOM	439	CD2 PHE G 210	17.460	-14.923	87.131	1.00	39.15	C
	ATOM	440	CE1 PHE G 210	15.765	-16.356	85.466	1.00	38.42	C
	ATOM	441	CE2 PHE G 210	17.960	-15.985	86.369	1.00	39.64	C
	ATOM	442	CZ PHE G 210	17.108	-16.704	85.540	1.00	38.39	C
	ATOM	443	N GLU G 211	14.201	-16.084	89.685	1.00	41.43	N
	ATOM	444	CA GLU G 211	14.537	-17.169	90.601	1.00	40.62	C
	ATOM	445	C GLU G 211	14.945	-18.405	89.815	1.00	39.25	C
	ATOM	446	O GLU G 211	14.389	-18.686	88.752	1.00	39.17	O
	ATOM	447	CB GLU G 211	13.377	-17.492	91.560	1.00	42.31	C
	ATOM	448	CG GLU G 211	12.269	-18.363	90.988	1.00	44.19	C
	ATOM	449	CD GLU G 211	11.492	-19.098	92.070	1.00	45.89	C
	ATOM	450	OE1 GLU G 211	12.108	-19.884	92.828	1.00	45.92	O
	ATOM	451	OE2 GLU G 211	10.261	-18.904	92.162	1.00	47.68	O
	ATOM	452	N PRO G 212	15.985	-19.110	90.284	1.00	38.52	N
	ATOM	453	CA PRO G 212	16.486	-20.322	89.626	1.00	36.21	C
	ATOM	454	C PRO G 212	15.734	-21.602	89.983	1.00	33.09	C
	ATOM	455	O PRO G 212	15.585	-21.959	91.154	1.00	32.86	O
	ATOM	456	CB PRO G 212	17.945	-20.369	90.077	1.00	37.50	C
	ATOM	457	CG PRO G 212	17.859	-19.845	91.481	1.00	38.90	C
	ATOM	458	CD PRO G 212	16.908	-18.665	91.347	1.00	38.66	C
	ATOM	459	N PRO G 212	15.777	-22.267	88.958	1.00	20.77	N

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FIG. 53-15	ATOM 461	C	ILE G 213	15.478	-24.612	88.691	1.00	24.26	C
	ATOM 462	O	ILE G 213	16.002	-24.562	87.576	1.00	25.13	O
	ATOM 463	CB	ILE G 213	13.235	-23.584	88.230	1.00	23.85	C
	ATOM 464	CG1	ILE G 213	12.002	-23.217	89.051	1.00	22.29	C
	ATOM 465	CG2	ILE G 213	13.020	-24.976	87.659	1.00	23.98	C
	ATOM 466	CD1	ILE G 213	11.675	-24.235	90.116	1.00	19.78	C
	ATOM 467	N	PRO G 214	15.785	-25.570	89.582	1.00	21.57	N
	ATOM 468	CA	PRO G 214	16.711	-26.636	89.203	1.00	19.74	C
	ATOM 469	C	PRO G 214	16.190	-27.279	87.923	1.00	19.30	C
	ATOM 470	O	PRO G 214	15.031	-27.701	87.850	1.00	19.65	O
	ATOM 471	CB	PRO G 214	16.616	-27.596	90.382	1.00	18.78	C
	ATOM 472	CG	PRO G 214	16.379	-26.697	91.512	1.00	20.57	C
	ATOM 473	CD	PRO G 214	15.341	-25.738	90.972	1.00	20.63	C
	ATOM 474	N	ILE G 215	17.011	-27.276	86.888	1.00	18.27	N
	ATOM 475	CA	ILE G 215	16.599	-27.855	85.633	1.00	19.05	C
	ATOM 476	C	ILE G 215	17.188	-29.253	85.428	1.00	21.00	C
	ATOM 477	O	ILE G 215	18.392	-29.474	85.572	1.00	21.46	O
	ATOM 478	CB	ILE G 215	16.939	-26.922	84.450	1.00	18.63	C
	ATOM 479	CG1	ILE G 215	18.449	-26.688	84.350	1.00	18.94	C
	ATOM 480	CG2	ILE G 215	16.207	-25.594	84.611	1.00	17.22	C
	ATOM 481	CD1	ILE G 215	18.865	-25.836	83.153	1.00	18.67	C
	ATOM 482	N	HIS G 216	16.314	-30.214	85.169	1.00	21.88	N
	ATOM 483	CA	HIS G 216	16.747	-31.572	84.933	1.00	22.93	C
	ATOM 484	C	HIS G 216	16.771	-31.766	83.424	1.00	23.43	C
	ATOM 485	O	HIS G 216	15.853	-31.323	82.734	1.00	23.56	O
	ATOM 486	CB	HIS G 216	15.762	-32.561	85.556	1.00	24.82	C
	ATOM 487	CG	HIS G 216	15.771	-32.576	87.052	1.00	28.60	C
	ATOM 488	ND1	HIS G 216	16.921	-32.414	87.793	1.00	31.33	N
	ATOM 489	CD2	HIS G 216	14.770	-32.751	87.945	1.00	30.95	C
	ATOM 490	CE1	HIS G 216	16.629	-32.492	89.080	1.00	32.29	C
	ATOM 491	NE2	HIS G 216	15.328	-32.696	89.200	1.00	32.75	N
	ATOM 492	N	TYR G 217	17.860	-32.320	82.901	1.00	22.34	N
	ATOM 493	CA	TYR G 217	17.939	-32.596	81.473	1.00	22.17	C
	ATOM 494	C	TYR G 217	17.934	-34.095	81.269	1.00	23.92	C
	ATOM 495	O	TYR G 217	18.844	-34.806	81.719	1.00	24.28	O
	ATOM 496	CB	TYR G 217	19.164	-31.957	80.839	1.00	20.79	C
	ATOM 497	CG	TYR G 217	18.885	-30.558	80.372	1.00	22.08	C
	ATOM 498	CD1	TYR G 217	17.960	-30.322	79.360	1.00	23.67	C
	ATOM 499	CD2	TYR G 217	19.496	-29.460	80.979	1.00	23.26	C
	ATOM 500	CE1	TYR G 217	17.638	-29.031	78.967	1.00	24.46	C
	ATOM 501	CE2	TYR G 217	19.179	-28.166	80.594	1.00	24.32	C
	ATOM 502	CZ	TYR G 217	18.247	-27.961	79.589	1.00	24.69	C
	ATOM 503	OH	TYR G 217	17.909	-26.690	79.227	1.00	24.29	O
	ATOM 504	N	CYS G 218	16.870	-34.575	80.641	1.00	24.27	N
	ATOM 505	CA	CYS G 218	16.695	-35.995	80.388	1.00	24.62	C
	ATOM 506	C	CYS G 218	17.113	-36.358	78.972	1.00	22.83	C
	ATOM 507	O	CYS G 218	17.567	-35.500	78.214	1.00	24.72	O
	ATOM 508	CB	CYS G 218	15.233	-36.354	80.639	1.00	26.38	C
	ATOM 509	SG	CYS G 218	14.704	-35.817	82.294	1.00	31.63	S
	ATOM 510	N	ALA G 219	16.974	-37.631	78.624	1.00	18.93	N
	ATOM 511	CA	ALA G 219	17.339	-38.109	77.294	1.00	16.07	C
	ATOM 512	C	ALA G 219	16.527	-37.448	76.171	1.00	13.63	C
	ATOM 513	O	ALA G 219	15.300	-37.319	76.257	1.00	13.39	O
	ATOM 514	CB	ALA G 219	17.195	-39.629	77.229	1.00	14.92	C
	ATOM 515	N	PRO G 220	17.219	-36.938	75.149	1.00	11.01	N
	ATOM 516	CA	PRO G 220	16.594	-36.283	74.001	1.00	11.11	C
	ATOM 517	C	PRO G 220	16.334	-37.262	72.860	1.00	13.18	C
	ATOM 518	O	PRO G 220	17.280	-37.698	72.182	1.00	13.29	O
	ATOM 519	CB	PRO G 220	17.643	-35.274	73.593	1.00	8.89	C
	ATOM 520	CG	PRO G 220	18.900	-36.045	73.827	1.00	7.54	C
	ATOM 521	CD	PRO G 220	18.667	-36.677	75.172	1.00	8.50	C
	ATOM 522	N	ALA G 221	15.061	-37.602	72.649	1.00	13.29	N
	ATOM 523	CA	ALA G 221	14.651	-38.512	71.579	1.00	12.43	C
	ATOM 524	C	ALA G 221	15.384	-39.856	71.586	1.00	13.18	C
	ATOM 525	O	ALA G 221	15.643	-40.442	72.651	1.00	14.79	O
	ATOM 526	CB	ALA G 221	14.820	-37.820	70.216	1.00	11.39	C
	ATOM 527	N	GLY G 222	15.702	-40.351	70.394	1.00	10.84	N
	ATOM 528	CA	GLY G 222	16.400	-41.612	70.290	1.00	11.36	C
	ATOM 529	C	GLY G 222	17.867	-41.511	70.656	1.00	9.70	C
	ATOM 530	O	GLY G 222	18.721	-41.016	69.861	1.00	10.63	O



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FIG. 53-16

ATOM	532	CA PHE G 223	19.496	-40.809	72.373	1.00	8.42	C
ATOM	533	C PHE G 223	19.456	-41.268	73.828	1.00	9.49	C
ATOM	534	O PHE G 223	18.366	-41.488	74.378	1.00	10.19	O
ATOM	535	CB PHE G 223	19.896	-39.331	72.344	1.00	10.62	C
ATOM	536	CG PHE G 223	20.232	-38.807	70.979	1.00	10.55	C
ATOM	537	CD1 PHE G 223	19.231	-38.447	70.084	1.00	11.49	C
ATOM	538	CD2 PHE G 223	21.560	-38.694	70.579	1.00	12.49	C
ATOM	539	CE1 PHE G 223	19.550	-37.980	68.805	1.00	12.26	C
ATOM	540	CE2 PHE G 223	21.892	-38.228	69.305	1.00	12.26	C
ATOM	541	CZ PHE G 223	20.884	-37.872	68.416	1.00	11.74	C
ATOM	542	N ALA G 224	20.622	-41.402	74.459	1.00	9.64	N
ATOM	543	CA ALA G 224	20.696	-41.822	75.860	1.00	12.19	C
ATOM	544	C ALA G 224	21.767	-41.039	76.600	1.00	14.07	C
ATOM	545	O ALA G 224	22.819	-40.756	76.040	1.00	16.11	O
ATOM	546	CB ALA G 224	20.991	-43.300	75.959	1.00	13.88	C
ATOM	547	N ILE G 225	21.489	-40.660	77.843	1.00	15.13	N
ATOM	548	CA ILE G 225	22.460	-39.919	78.636	1.00	16.80	C
ATOM	549	C ILE G 225	23.354	-40.919	79.359	1.00	17.78	C
ATOM	550	O ILE G 225	22.861	-41.867	79.972	1.00	17.14	O
ATOM	551	CB ILE G 225	21.776	-38.988	79.680	1.00	16.89	C
ATOM	552	CG1 ILE G 225	20.894	-37.961	78.974	1.00	17.32	C
ATOM	553	CG2 ILE G 225	22.823	-38.241	80.499	1.00	15.61	C
ATOM	554	CD1 ILE G 225	20.244	-36.988	79.911	1.00	18.48	C
ATOM	555	N LEU G 226	24.665	-40.714	79.265	1.00	19.57	N
ATOM	556	CA LEU G 226	25.647	-41.586	79.909	1.00	20.91	C
ATOM	557	C LEU G 226	26.440	-40.841	80.973	1.00	24.07	C
ATOM	558	O LEU G 226	27.391	-40.125	80.655	1.00	25.41	O
ATOM	559	CB LEU G 226	26.626	-42.145	78.877	1.00	18.80	C
ATOM	560	CG LEU G 226	26.421	-43.565	78.356	1.00	17.77	C
ATOM	561	CD1 LEU G 226	25.136	-43.665	77.576	1.00	18.13	C
ATOM	562	CD2 LEU G 226	27.594	-43.943	77.483	1.00	18.28	C
ATOM	563	N LYS G 227	26.073	-41.037	82.237	1.00	26.52	N
ATOM	564	CA LYS G 227	26.762	-40.383	83.342	1.00	27.94	C
ATOM	565	C LYS G 227	28.046	-41.125	83.675	1.00	29.17	C
ATOM	566	O LYS G 227	28.042	-42.351	83.782	1.00	28.73	O
ATOM	567	CB LYS G 227	25.871	-40.345	84.596	1.00	27.90	C
ATOM	568	CG LYS G 227	26.571	-39.821	85.871	1.00	29.64	C
ATOM	569	CD LYS G 227	25.679	-39.912	87.113	1.00	32.29	C
ATOM	570	CE LYS G 227	24.456	-39.001	86.999	1.00	34.48	C
ATOM	571	NZ LYS G 227	23.364	-39.285	87.981	1.00	34.38	N
ATOM	572	N CYS G 228	29.156	-40.402	83.769	1.00	30.76	N
ATOM	573	CA CYS G 228	30.406	-41.034	84.164	1.00	31.72	C
ATOM	574	C CYS G 228	30.354	-41.009	85.688	1.00	31.86	C
ATOM	575	O CYS G 228	30.128	-39.947	86.288	1.00	31.34	O
ATOM	576	CB CYS G 228	31.630	-40.254	83.684	1.00	32.88	C
ATOM	577	SG CYS G 228	33.191	-41.021	84.247	1.00	35.47	S
ATOM	578	N ASN G 229	30.543	-42.169	86.307	1.00	32.07	N
ATOM	579	CA ASN G 229	30.487	-42.279	87.761	1.00	32.72	C
ATOM	580	C ASN G 229	31.832	-42.135	88.457	1.00	34.60	C
ATOM	581	O ASN G 229	31.911	-42.205	89.686	1.00	35.58	O
ATOM	582	CB ASN G 229	29.826	-43.590	88.153	1.00	29.60	C
ATOM	583	CG ASN G 229	28.562	-43.849	87.372	1.00	27.66	C
ATOM	584	OD1 ASN G 229	28.577	-44.573	86.383	1.00	29.57	O
ATOM	585	ND2 ASN G 229	27.465	-43.236	87.788	1.00	25.67	N
ATOM	586	N ASN G 230	32.894	-41.963	87.676	1.00	36.32	N
ATOM	587	CA ASN G 230	34.235	-41.791	88.233	1.00	38.29	C
ATOM	588	C ASN G 230	34.178	-40.551	89.128	1.00	39.43	C
ATOM	589	O ASN G 230	34.082	-39.421	88.631	1.00	40.23	O
ATOM	590	CB ASN G 230	35.249	-41.587	87.101	1.00	39.40	C
ATOM	591	CG ASN G 230	36.676	-41.423	87.602	1.00	41.01	C
ATOM	592	OD1 ASN G 230	36.909	-41.063	88.758	1.00	42.26	O
ATOM	593	ND2 ASN G 230	37.641	-41.688	86.730	1.00	41.03	N
ATOM	594	N LYS G 231	34.212	-40.776	90.442	1.00	39.89	N
ATOM	595	CA LYS G 231	34.130	-39.706	91.447	1.00	39.44	C
ATOM	596	C LYS G 231	34.979	-38.480	91.139	1.00	38.08	C
ATOM	597	O LYS G 231	34.615	-37.360	91.500	1.00	36.75	O
ATOM	598	CB LYS G 231	34.504	-40.238	92.835	1.00	41.08	C
ATOM	599	CG LYS G 231	35.963	-40.671	92.968	1.00	44.34	C
ATOM	600	CD LYS G 231	36.306	-41.090	94.396	1.00	45.89	C
ATOM	601	CE LYS G 231	37.782	-41.470	94.521	1.00	47.71	C

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FIG. 53-17	ATOM	603	N	THR G 232	36.099 -38.700 90.460 1.00 37.10	N
	ATOM	604	CA	THR G 232	37.012 -37.625 90.110 1.00 36.36	C
	ATOM	605	C	THR G 232	37.277 -37.596 88.605 1.00 36.66	C
	ATOM	606	O	THR G 232	38.435 -37.552 88.169 1.00 37.42	O
	ATOM	607	CB	THR G 232	38.345 -37.802 90.840 1.00 35.93	C
	ATOM	608	OG1	THR G 232	38.102 -38.234 92.189 1.00 35.22	O
	ATOM	609	CG2	THR G 232	39.117 -36.492 90.861 1.00 37.20	C
	ATOM	610	N	PHE G 233	36.217 -37.654 87.802 1.00 35.64	N
	ATOM	611	CA	PHE G 233	36.398 -37.616 86.357 1.00 34.71	C
	ATOM	612	C	PHE G 233	36.969 -36.249 86.011 1.00 34.94	C
	ATOM	613	O	PHE G 233	36.451 -35.214 86.442 1.00 35.73	O
	ATOM	614	CB	PHE G 233	35.078 -37.847 85.622 1.00 33.02	C
	ATOM	615	CG	PHE G 233	35.241 -38.061 84.142 1.00 29.97	C
	ATOM	616	CD1	PHE G 233	36.468 -38.461 83.612 1.00 28.03	C
	ATOM	617	CD2	PHE G 233	34.174 -37.856 83.279 1.00 27.59	C
	ATOM	618	CE1	PHE G 233	36.625 -38.650 82.250 1.00 27.32	C
	ATOM	619	CE2	PHE G 233	34.322 -38.043 81.919 1.00 26.38	C
	ATOM	620	CZ	PHE G 233	35.547 -38.440 81.400 1.00 26.71	C
	ATOM	621	N	ASN G 234	38.033 -36.247 85.225 1.00 34.87	N
	ATOM	622	CA	ASN G 234	38.697 -35.012 84.873 1.00 35.27	C
	ATOM	623	C	ASN G 234	38.655 -34.658 83.394 1.00 35.04	C
	ATOM	624	O	ASN G 234	39.563 -34.971 82.630 1.00 33.89	O
	ATOM	625	CB	ASN G 234	40.123 -35.058 85.422 1.00 38.76	C
	ATOM	626	CG	ASN G 234	40.998 -33.931 84.914 1.00 42.99	C
	ATOM	627	OD1	ASN G 234	40.748 -32.752 85.180 1.00 42.47	O
	ATOM	628	ND2	ASN G 234	42.059 -34.309 84.204 1.00 47.05	N
	ATOM	629	N	GLY G 235	37.541 -34.047 83.007 1.00 36.12	N
	ATOM	630	CA	GLY G 235	37.333 -33.596 81.643 1.00 36.47	C
	ATOM	631	C	GLY G 235	37.286 -34.625 80.532 1.00 37.20	C
	ATOM	632	O	GLY G 235	36.373 -35.448 80.450 1.00 36.74	O
	ATOM	633	N	THR G 236	38.265 -34.517 79.643 1.00 38.34	N
	ATOM	634	CA	THR G 236	38.400 -35.386 78.484 1.00 38.15	C
	ATOM	635	C	THR G 236	39.055 -36.704 78.885 1.00 37.90	C
	ATOM	636	O	THR G 236	39.874 -36.744 79.805 1.00 37.08	O
	ATOM	637	CB	THR G 236	39.275 -34.700 77.416 1.00 37.38	C
	ATOM	638	OG1	THR G 236	38.882 -33.327 77.293 1.00 38.47	O
	ATOM	639	CG2	THR G 236	39.130 -35.379 76.069 1.00 36.15	C
	ATOM	640	N	GLY G 237	38.685 -37.781 78.201 1.00 38.40	N
	ATOM	641	CA	GLY G 237	39.278 -39.068 78.504 1.00 38.38	C
	ATOM	642	C	GLY G 237	38.295 -40.218 78.510 1.00 39.07	C
	ATOM	643	O	GLY G 237	37.075 -40.016 78.501 1.00 38.90	O
	ATOM	644	N	PRO G 238	38.809 -41.456 78.508 1.00 39.11	N
	ATOM	645	CA	PRO G 238	37.973 -42.653 78.513 1.00 39.26	C
	ATOM	646	C	PRO G 238	37.466 -42.981 79.913 1.00 39.29	C
	ATOM	647	O	PRO G 238	38.191 -43.555 80.733 1.00 39.99	O
	ATOM	648	CB	PRO G 238	38.924 -43.722 77.981 1.00 39.01	C
	ATOM	649	CG	PRO G 238	40.222 -43.310 78.557 1.00 38.17	C
	ATOM	650	CD	PRO G 238	40.231 -41.811 78.355 1.00 38.34	C
	ATOM	651	N	CYS G 239	36.240 -42.559 80.205 1.00 38.74	N
	ATOM	652	CA	CYS G 239	35.639 -42.827 81.502 1.00 37.11	C
	ATOM	653	C	CYS G 239	35.481 -44.330 81.670 1.00 36.78	C
	ATOM	654	O	CYS G 239	34.889 -45.002 80.824 1.00 36.13	O
	ATOM	655	CB	CYS G 239	34.269 -42.156 81.622 1.00 36.43	C
	ATOM	656	SG	CYS G 239	33.333 -42.688 83.095 1.00 34.24	S
	ATOM	657	N	THR G 240	36.023 -44.853 82.761 1.00 37.49	N
	ATOM	658	CA	THR G 240	35.931 -46.274 83.050 1.00 37.98	C
	ATOM	659	C	THR G 240	34.533 -46.598 83.586 1.00 37.13	C
	ATOM	660	O	THR G 240	33.684 -47.130 82.868 1.00 37.18	O
	ATOM	661	CB	THR G 240	37.003 -46.699 84.081 1.00 39.11	C
	ATOM	662	OG1	THR G 240	37.034 -45.752 85.157 1.00 39.76	O
	ATOM	663	CG2	THR G 240	38.379 -46.767 83.430 1.00 39.56	C
	ATOM	664	N	ASN G 241	34.291 -46.228 84.839 1.00 36.08	N
	ATOM	665	CA	ASN G 241	33.013 -46.457 85.494 1.00 35.12	C
	ATOM	666	C	ASN G 241	31.985 -45.476 84.924 1.00 34.97	C
	ATOM	667	O	ASN G 241	32.108 -44.266 85.120 1.00 35.71	O
	ATOM	668	CB	ASN G 241	33.185 -46.253 87.001 1.00 34.78	C
	ATOM	669	CG	ASN G 241	31.956 -46.648 87.795 1.00 35.17	C
	ATOM	670	OD1	ASN G 241	30.847 -46.703 87.262 1.00 35.56	O
	ATOM	671	ND2	ASN G 241	32.149 -46.926 89.081 1.00 33.79	N
	ATOM	672	N	VAL G 242	30.983 -45.997 84.771 1.00 34.43	N

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FIG. 53-18

ATOM 674	C VAL G 242	28.633 -45.926 83.469 1.00 34.85	C
ATOM 675	O VAL G 242	28.630 -47.158 83.403 1.00 35.99	O
ATOM 676	CB VAL G 242	30.401 -44.674 82.193 1.00 34.41	C
ATOM 677	CG1 VAL G 242	30.835 -45.841 81.336 1.00 34.06	C
ATOM 678	CG2 VAL G 242	29.284 -43.929 81.506 1.00 35.80	C
ATOM 679	N SER G 243	27.520 -45.197 83.422 1.00 34.24	N
ATOM 680	CA SER G 243	26.202 -45.814 83.306 1.00 33.06	C
ATOM 681	C SER G 243	25.149 -44.908 82.678 1.00 31.78	C
ATOM 682	O SER G 243	25.223 -43.680 82.779 1.00 32.45	O
ATOM 683	CB SER G 243	25.730 -46.294 84.682 1.00 34.26	C
ATOM 684	OG SER G 243	25.920 -45.301 85.680 1.00 34.99	O
ATOM 685	N THR G 244	24.178 -45.523 82.013 1.00 29.73	N
ATOM 686	CA THR G 244	23.100 -44.794 81.366 1.00 29.06	C
ATOM 687	C THR G 244	22.137 -44.262 82.415 1.00 29.76	C
ATOM 688	O THR G 244	21.936 -44.894 83.446 1.00 29.94	O
ATOM 689	CB THR G 244	22.337 -45.694 80.375 1.00 28.55	C
ATOM 690	OG1 THR G 244	23.162 -45.975 79.238 1.00 27.22	O
ATOM 691	CG2 THR G 244	21.073 -45.021 79.906 1.00 30.50	C
ATOM 692	N VAL G 245	21.581 -43.079 82.162 1.00 30.22	N
ATOM 693	CA VAL G 245	20.629 -42.439 83.068 1.00 28.10	C
ATOM 694	C VAL G 245	19.507 -41.832 82.244 1.00 27.35	C
ATOM 695	O VAL G 245	19.677 -41.544 81.056 1.00 26.22	O
ATOM 696	CB VAL G 245	21.281 -41.312 83.919 1.00 26.91	C
ATOM 697	CG1 VAL G 245	22.250 -41.890 84.926 1.00 28.47	C
ATOM 698	CG2 VAL G 245	22.000 -40.321 83.036 1.00 26.25	C
ATOM 699	N GLN G 246	18.352 -41.661 82.874 1.00 27.28	N
ATOM 700	CA GLN G 246	17.197 -41.086 82.202 1.00 28.75	C
ATOM 701	C GLN G 246	17.335 -39.566 82.151 1.00 29.05	C
ATOM 702	O GLN G 246	16.933 -38.930 81.174 1.00 28.66	O
ATOM 703	CB GLN G 246	15.913 -41.469 82.934 1.00 30.26	C
ATOM 704	CG GLN G 246	14.656 -41.135 82.163 1.00 33.92	C
ATOM 705	CD GLN G 246	14.473 -42.015 80.944 1.00 35.79	C
ATOM 706	OE1 GLN G 246	14.017 -43.155 81.053 1.00 37.71	O
ATOM 707	NE2 GLN G 246	14.820 -41.489 79.772 1.00 35.44	N
ATOM 708	N CYS G 247	17.900 -38.997 83.215 1.00 29.31	N
ATOM 709	CA CYS G 247	18.125 -37.556 83.317 1.00 29.67	C
ATOM 710	C CYS G 247	19.424 -37.342 84.095 1.00 28.79	C
ATOM 711	O CYS G 247	19.809 -38.184 84.910 1.00 29.02	O
ATOM 712	CB CYS G 247	16.966 -36.870 84.053 1.00 30.99	C
ATOM 713	SG CYS G 247	15.297 -37.346 83.488 1.00 32.88	S
ATOM 714	N THR G 248	20.087 -36.215 83.840 1.00 27.61	N
ATOM 715	CA THR G 248	21.350 -35.860 84.490 1.00 25.20	C
ATOM 716	C THR G 248	21.286 -35.759 86.025 1.00 23.90	C
ATOM 717	O THR G 248	21.641 -36.718 86.732 1.00 25.55	O
ATOM 718	CB THR G 248	21.897 -34.551 83.898 1.00 24.29	C
ATOM 719	OG1 THR G 248	20.890 -33.533 83.968 1.00 24.48	O
ATOM 720	CG2 THR G 248	22.282 -34.758 82.444 1.00 23.90	C
ATOM 721	N HIS G 249	20.923 -34.581 86.526 1.00 21.13	N
ATOM 722	CA HIS G 249	20.779 -34.311 87.960 1.00 19.07	C
ATOM 723	C HIS G 249	20.168 -32.918 88.142 1.00 16.85	C
ATOM 724	O HIS G 249	19.735 -32.307 87.161 1.00 15.06	O
ATOM 725	CB HIS G 249	22.104 -34.470 88.738 1.00 21.24	C
ATOM 726	CG HIS G 249	23.159 -33.461 88.399 1.00 21.64	C
ATOM 727	ND1 HIS G 249	23.445 -33.112 87.106 1.00 23.08	N
ATOM 728	CD2 HIS G 249	24.025 -32.825 89.232 1.00 21.09	C
ATOM 729	CE1 HIS G 249	24.467 -32.282 87.173 1.00 23.31	C
ATOM 730	NE2 HIS G 249	24.853 -32.079 88.439 1.00 20.74	N
ATOM 731	N GLY G 250	20.029 -32.462 89.386 1.00 13.85	N
ATOM 732	CA GLY G 250	19.436 -31.154 89.630 1.00 11.77	C
ATOM 733	C GLY G 250	20.382 -30.011 89.355 1.00 9.55	C
ATOM 734	O GLY G 250	21.061 -29.553 90.265 1.00 7.84	O
ATOM 735	N ILE G 251	20.371 -29.512 88.122 1.00 8.82	N
ATOM 736	CA ILE G 251	21.274 -28.447 87.718 1.00 10.81	C
ATOM 737	C ILE G 251	20.680 -27.060 87.930 1.00 13.34	C
ATOM 738	O ILE G 251	19.649 -26.739 87.351 1.00 14.54	O
ATOM 739	CB ILE G 251	21.630 -28.564 86.220 1.00 9.66	C
ATOM 740	CG1 ILE G 251	21.804 -30.025 85.810 1.00 10.10	C
ATOM 741	CG2 ILE G 251	22.922 -27.827 85.932 1.00 11.25	C
ATOM 742	CD1 ILE G 251	21.969 -30.217 84.306 1.00 10.97	C
ATOM 743	N ARG G 252	21.310 -26.242 88.762 1.00 14.65	N

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FIG. 53-19	ATOM 745	C ARG G 252	21.536	-23.902	88.040	1.00	15.18	C
	ATOM 746	O ARG G 252	22.729	-23.612	88.184	1.00	14.72	O
	ATOM 747	CB ARG G 252	21.089	-24.447	90.437	1.00	16.34	C
	ATOM 748	CG ARG G 252	19.816	-24.400	91.267	1.00	18.59	C
	ATOM 749	CD ARG G 252	20.048	-23.675	92.571	1.00	20.27	C
	ATOM 750	NE ARG G 252	21.125	-24.274	93.352	1.00	21.75	N
	ATOM 751	CZ ARG G 252	21.095	-24.399	94.671	1.00	22.91	C
	ATOM 752	NH1 ARG G 252	20.035	-23.967	95.347	1.00	23.31	N
	ATOM 753	NH2 ARG G 252	22.125	-24.947	95.307	1.00	23.29	N
	ATOM 754	N PRO G 253	20.794	-23.380	87.050	1.00	14.19	N
	ATOM 755	CA PRO G 253	21.369	-22.446	86.082	1.00	15.88	C
	ATOM 756	C PRO G 253	21.631	-21.059	86.659	1.00	17.45	C
	ATOM 757	O PRO G 253	20.769	-20.184	86.640	1.00	18.70	O
	ATOM 758	CB PRO G 253	20.320	-22.430	84.978	1.00	15.49	C
	ATOM 759	CG PRO G 253	19.040	-22.604	85.746	1.00	14.37	C
	ATOM 760	CD PRO G 253	19.391	-23.683	86.722	1.00	13.38	C
	ATOM 761	N VAL G 254	22.821	-20.868	87.205	1.00	17.92	N
	ATOM 762	CA VAL G 254	23.166	-19.583	87.786	1.00	17.08	C
	ATOM 763	C VAL G 254	24.073	-18.852	86.828	1.00	16.36	C
	ATOM 764	O VAL G 254	25.088	-19.396	86.392	1.00	18.64	O
	ATOM 765	CB VAL G 254	23.897	-19.744	89.135	1.00	18.77	C
	ATOM 766	CG1 VAL G 254	24.303	-18.376	89.680	1.00	20.07	C
	ATOM 767	CG2 VAL G 254	23.013	-20.485	90.136	1.00	15.73	C
	ATOM 768	N VAL G 255	23.654	-17.660	86.423	1.00	13.80	N
	ATOM 769	CA VAL G 255	24.459	-16.842	85.528	1.00	11.88	C
	ATOM 770	C VAL G 255	25.293	-15.902	86.398	1.00	11.33	C
	ATOM 771	O VAL G 255	24.753	-15.203	87.265	1.00	11.59	O
	ATOM 772	CB VAL G 255	23.582	-16.030	84.582	1.00	11.26	C
	ATOM 773	CG1 VAL G 255	24.422	-14.993	83.857	1.00	12.22	C
	ATOM 774	CG2 VAL G 255	22.905	-16.957	83.591	1.00	8.16	C
	ATOM 775	N SER G 256	26.602	-15.900	86.184	1.00	9.34	N
	ATOM 776	CA SER G 256	27.488	-15.065	86.974	1.00	9.65	C
	ATOM 777	C SER G 256	28.901	-15.234	86.447	1.00	8.51	C
	ATOM 778	O SER G 256	29.167	-16.172	85.692	1.00	7.45	O
	ATOM 779	CB SER G 256	27.416	-15.499	88.440	1.00	11.83	C
	ATOM 780	OG SER G 256	27.666	-16.894	88.563	1.00	16.05	O
	ATOM 781	N THR G 257	29.806	-14.344	86.849	1.00	6.62	N
	ATOM 782	CA THR G 257	31.186	-14.409	86.388	1.00	7.04	C
	ATOM 783	C THR G 257	32.209	-14.728	87.463	1.00	8.38	C
	ATOM 784	O THR G 257	31.963	-14.529	88.654	1.00	6.92	O
	ATOM 785	CB THR G 257	31.596	-13.104	85.702	1.00	6.93	C
	ATOM 786	OG1 THR G 257	31.300	-11.999	86.574	1.00	6.69	O
	ATOM 787	CG2 THR G 257	30.855	-12.950	84.386	1.00	4.16	C
	ATOM 788	N GLN G 258	33.377	-15.190	87.010	1.00	10.72	N
	ATOM 789	CA GLN G 258	34.517	-15.569	87.852	1.00	13.00	C
	ATOM 790	C GLN G 258	34.282	-16.449	89.076	1.00	13.60	C
	ATOM 791	O GLN G 258	35.225	-17.050	89.590	1.00	12.26	O
	ATOM 792	CB GLN G 258	35.425	-14.360	88.187	1.00	16.33	C
	ATOM 793	CG GLN G 258	34.769	-13.073	88.686	1.00	18.73	C
	ATOM 794	CD GLN G 258	35.736	-11.885	88.689	1.00	22.36	C
	ATOM 795	OE1 GLN G 258	36.009	-11.297	89.730	1.00	26.27	O
	ATOM 796	NE2 GLN G 258	36.249	-11.530	87.522	1.00	22.75	N
	ATOM 797	N LEU G 259	33.025	-16.608	89.482	1.00	14.36	N
	ATOM 798	CA LEU G 259	32.687	-17.423	90.637	1.00	14.56	C
	ATOM 799	C LEU G 259	31.411	-18.193	90.312	1.00	15.43	C
	ATOM 800	O LEU G 259	30.372	-17.603	90.038	1.00	14.37	O
	ATOM 801	CB LEU G 259	32.468	-16.553	91.885	1.00	13.53	C
	ATOM 802	CG LEU G 259	33.520	-15.542	92.381	1.00	14.36	C
	ATOM 803	CD1 LEU G 259	32.979	-14.812	93.598	1.00	13.95	C
	ATOM 804	CD2 LEU G 259	34.834	-16.214	92.727	1.00	12.89	C
	ATOM 805	N LEU G 260	31.544	-19.514	90.233	1.00	17.80	N
	ATOM 806	CA LEU G 260	30.426	-20.411	89.967	1.00	16.61	C
	ATOM 807	C LEU G 260	29.751	-20.526	91.328	1.00	16.85	C
	ATOM 808	O LEU G 260	30.418	-20.767	92.343	1.00	16.91	O
	ATOM 809	CB LEU G 260	30.944	-21.777	89.505	1.00	15.05	C
	ATOM 810	CG LEU G 260	31.548	-21.902	88.103	1.00	12.93	C
	ATOM 811	CD1 LEU G 260	32.443	-23.115	88.006	1.00	9.99	C
	ATOM 812	CD2 LEU G 260	30.436	-21.995	87.083	1.00	14.84	C
	ATOM 813	N LEU G 261	28.438	-20.355	91.357	1.00	16.28	N
	ATOM 814	CA LEU G 261	27.714	-20.387	92.610	1.00	15.45	C

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FIG. 53-20

ATOM	816	O	LEU	G	261	26.055	-21.719	91.530	1.00	15.07	O
ATOM	817	CB	LEU	G	261	27.155	-18.994	92.941	1.00	15.44	C
ATOM	818	CG	LEU	G	261	27.903	-17.709	92.562	1.00	14.64	C
ATOM	819	CD1	LEU	G	261	26.995	-16.531	92.836	1.00	15.56	C
ATOM	820	CD2	LEU	G	261	29.208	-17.580	93.328	1.00	14.51	C
ATOM	821	N	ASN	G	262	26.091	-21.722	93.795	1.00	14.73	N
ATOM	822	CA	ASN	G	262	24.955	-22.617	93.986	1.00	15.35	C
ATOM	823	C	ASN	G	262	24.966	-23.881	93.128	1.00	16.77	C
ATOM	824	O	ASN	G	262	23.895	-24.406	92.778	1.00	14.61	O
ATOM	825	CB	ASN	G	262	23.655	-21.840	93.763	1.00	13.25	C
ATOM	826	CG	ASN	G	262	23.276	-21.004	94.953	1.00	14.34	C
ATOM	827	OD1	ASN	G	262	24.149	-20.476	95.649	1.00	13.74	O
ATOM	828	ND2	ASN	G	262	21.974	-20.958	95.249	1.00	19.13	N
ATOM	829	N	GLY	G	263	26.162	-24.430	92.910	1.00	18.74	N
ATOM	830	CA	GLY	G	263	26.297	-25.613	92.070	1.00	20.11	C
ATOM	831	C	GLY	G	263	26.893	-26.866	92.695	1.00	20.38	C
ATOM	832	O	GLY	G	263	26.976	-26.990	93.918	1.00	18.64	O
ATOM	833	N	SER	G	264	27.340	-27.783	91.839	1.00	22.57	N
ATOM	834	CA	SER	G	264	27.920	-29.055	92.272	1.00	24.43	C
ATOM	835	C	SER	G	264	29.383	-28.986	92.685	1.00	24.80	C
ATOM	836	O	SER	G	264	30.222	-28.469	91.947	1.00	26.75	O
ATOM	837	CB	SER	G	264	27.731	-30.114	91.181	1.00	24.18	C
ATOM	838	OG	SER	G	264	28.390	-31.332	91.492	1.00	25.32	O
ATOM	839	N	LEU	G	265	29.679	-29.569	93.842	1.00	24.24	N
ATOM	840	CA	LEU	G	265	31.026	-29.599	94.405	1.00	24.88	C
ATOM	841	C	LEU	G	265	31.707	-30.915	94.056	1.00	26.63	C
ATOM	842	O	LEU	G	265	31.068	-31.863	93.581	1.00	28.11	O
ATOM	843	CB	LEU	G	265	30.971	-29.520	95.936	1.00	23.01	C
ATOM	844	CG	LEU	G	265	30.425	-28.329	96.727	1.00	21.06	C
ATOM	845	CD1	LEU	G	265	30.318	-28.728	98.173	1.00	19.70	C
ATOM	846	CD2	LEU	G	265	31.333	-27.131	96.597	1.00	19.59	C
ATOM	847	N	ALA	G	266	33.006	-30.980	94.321	1.00	26.39	N
ATOM	848	CA	ALA	G	266	33.755	-32.200	94.089	1.00	27.04	C
ATOM	849	C	ALA	G	266	33.572	-33.011	95.364	1.00	28.11	C
ATOM	850	O	ALA	G	266	33.583	-32.463	96.472	1.00	26.76	O
ATOM	851	CB	ALA	G	266	35.224	-31.898	93.860	1.00	26.32	C
ATOM	852	N	GLU	G	267	33.364	-34.313	95.216	1.00	30.45	N
ATOM	853	CA	GLU	G	267	33.183	-35.150	96.390	1.00	31.74	C
ATOM	854	C	GLU	G	267	34.493	-35.663	96.959	1.00	31.08	C
ATOM	855	O	GLU	G	267	34.528	-36.149	98.087	1.00	31.50	O
ATOM	856	CB	GLU	G	267	32.215	-36.296	96.108	1.00	33.74	C
ATOM	857	CG	GLU	G	267	32.572	-37.169	94.930	1.00	36.70	C
ATOM	858	CD	GLU	G	267	31.470	-38.154	94.615	1.00	38.49	C
ATOM	859	OE1	GLU	G	267	30.287	-37.741	94.642	1.00	38.38	O
ATOM	860	OE2	GLU	G	267	31.781	-39.336	94.346	1.00	40.34	O
ATOM	861	N	GLU	G	268	35.569	-35.537	96.193	1.00	30.63	N
ATOM	862	CA	GLU	G	268	36.871	-35.993	96.661	1.00	31.06	C
ATOM	863	C	GLU	G	268	37.859	-34.887	96.982	1.00	30.70	C
ATOM	864	O	GLU	G	268	38.087	-34.567	98.149	1.00	31.59	O
ATOM	865	CB	GLU	G	268	37.475	-36.972	95.666	1.00	30.64	C
ATOM	866	CG	GLU	G	268	37.182	-38.400	96.033	1.00	32.42	C
ATOM	867	CD	GLU	G	268	37.983	-38.864	97.234	1.00	34.32	C
ATOM	868	OE1	GLU	G	268	39.142	-39.287	97.039	1.00	33.80	O
ATOM	869	OE2	GLU	G	268	37.446	-38.823	98.359	1.00	36.47	O
ATOM	870	N	GLU	G	269	38.475	-34.330	95.947	1.00	29.74	N
ATOM	871	CA	GLU	G	269	39.443	-33.259	96.116	1.00	28.78	C
ATOM	872	C	GLU	G	269	39.107	-32.188	95.099	1.00	27.43	C
ATOM	873	O	GLU	G	269	38.184	-32.356	94.296	1.00	26.47	O
ATOM	874	CB	GLU	G	269	40.858	-33.767	95.847	1.00	30.51	C
ATOM	875	CG	GLU	G	269	41.339	-34.857	96.781	1.00	34.12	C
ATOM	876	CD	GLU	G	269	42.556	-35.568	96.235	1.00	37.29	C
ATOM	877	OE1	GLU	G	269	42.376	-36.543	95.470	1.00	38.77	O
ATOM	878	OE2	GLU	G	269	43.688	-35.132	96.539	1.00	38.33	O
ATOM	879	N	VAL	G	270	39.863	-31.093	95.133	1.00	25.65	N
ATOM	880	CA	VAL	G	270	39.665	-29.995	94.199	1.00	22.37	C
ATOM	881	C	VAL	G	270	40.100	-30.507	92.830	1.00	20.77	C
ATOM	882	O	VAL	G	270	41.216	-31.019	92.677	1.00	21.12	O
ATOM	883	CB	VAL	G	270	40.524	-28.759	94.579	1.00	21.80	C
ATOM	884	CG1	VAL	G	270	40.193	-27.581	93.666	1.00	19.80	C
ATOM	885	CG2	VAL	G	270	40.200	-28.378	96.035	1.00	21.76	C

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FIG. 53-21	ATOM	887	CA	VAL G 271	39.487	-30.856	90.500	1.00	15.81	C
	ATOM	888	C	VAL G 271	39.389	-29.664	89.562	1.00	15.48	C
	ATOM	889	O	VAL G 271	38.424	-28.910	89.618	1.00	15.34	O
	ATOM	890	CB	VAL G 271	38.475	-31.916	90.036	1.00	14.93	C
	ATOM	891	CG1	VAL G 271	38.854	-32.436	88.652	1.00	16.36	C
	ATOM	892	CG2	VAL G 271	38.413	-33.050	91.031	1.00	12.91	C
	ATOM	893	N	ILE G 272	40.387	-29.500	88.703	1.00	14.98	N
	ATOM	894	CA	ILE G 272	40.418	-28.402	87.744	1.00	15.27	C
	ATOM	895	C	ILE G 272	40.249	-29.029	86.367	1.00	14.98	C
	ATOM	896	O	ILE G 272	40.471	-30.223	86.202	1.00	17.63	O
	ATOM	897	CB	ILE G 272	41.765	-27.619	87.822	1.00	15.43	C
	ATOM	898	CG1	ILE G 272	42.943	-28.550	87.501	1.00	15.65	C
	ATOM	899	CG2	ILE G 272	41.930	-26.992	89.211	1.00	14.26	C
	ATOM	900	CD1	ILE G 272	44.307	-27.944	87.724	1.00	13.52	C
	ATOM	901	N	ARG G 273	39.839	-28.240	85.386	1.00	13.53	N
	ATOM	902	CA	ARG G 273	39.633	-28.743	84.039	1.00	12.31	C
	ATOM	903	C	ARG G 273	39.828	-27.640	83.000	1.00	13.14	C
	ATOM	904	O	ARG G 273	39.500	-26.476	83.241	1.00	12.25	O
	ATOM	905	CB	ARG G 273	38.244	-29.381	83.925	1.00	11.20	C
	ATOM	906	CG	ARG G 273	38.204	-30.836	84.392	1.00	12.42	C
	ATOM	907	CD	ARG G 273	36.795	-31.387	84.533	1.00	7.85	C
	ATOM	908	NE	ARG G 273	36.151	-30.834	85.711	1.00	8.24	N
	ATOM	909	CZ	ARG G 273	35.797	-31.538	86.786	1.00	6.73	C
	ATOM	910	NH1	ARG G 273	36.011	-32.851	86.846	1.00	2.00	N
	ATOM	911	NH2	ARG G 273	35.297	-30.898	87.839	1.00	6.75	N
	ATOM	912	N	SER G 274	40.421	-28.008	81.866	1.00	14.05	N
	ATOM	913	CA	SER G 274	40.685	-27.083	80.771	1.00	14.41	C
	ATOM	914	C	SER G 274	40.862	-27.881	79.498	1.00	16.49	C
	ATOM	915	O	SER G 274	41.250	-29.051	79.541	1.00	16.60	O
	ATOM	916	CB	SER G 274	41.959	-26.295	81.019	1.00	13.52	C
	ATOM	917	OG	SER G 274	42.300	-25.536	79.866	1.00	14.72	O
	ATOM	918	N	VAL G 275	40.588	-27.239	78.365	1.00	18.87	N
	ATOM	919	CA	VAL G 275	40.713	-27.881	77.061	1.00	20.86	C
	ATOM	920	C	VAL G 275	42.171	-28.111	76.797	1.00	21.77	C
	ATOM	921	O	VAL G 275	42.571	-29.156	76.288	1.00	22.15	O
	ATOM	922	CB	VAL G 275	40.208	-26.977	75.912	1.00	22.43	C
	ATOM	923	CG1	VAL G 275	40.314	-27.704	74.579	1.00	21.35	C
	ATOM	924	CG2	VAL G 275	38.784	-26.540	76.158	1.00	23.72	C
	ATOM	925	N	ASN G 276	42.968	-27.115	77.163	1.00	23.25	N
	ATOM	926	CA	ASN G 276	44.404	-27.151	76.937	1.00	23.21	C
	ATOM	927	C	ASN G 276	45.032	-26.306	78.024	1.00	22.58	C
	ATOM	928	O	ASN G 276	44.917	-25.081	77.997	1.00	23.34	O
	ATOM	929	CB	ASN G 276	44.690	-26.511	75.582	1.00	24.97	C
	ATOM	930	CG	ASN G 276	46.021	-26.925	74.999	1.00	26.93	C
	ATOM	931	OD1	ASN G 276	47.022	-27.103	75.710	1.00	26.46	O
	ATOM	932	ND2	ASN G 276	46.025	-27.059	73.678	1.00	27.04	N
	ATOM	933	N	PHE G 277	45.652	-26.961	78.999	1.00	21.99	N
	ATOM	934	CA	PHE G 277	46.296	-26.265	80.110	1.00	21.09	C
	ATOM	935	C	PHE G 277	47.529	-25.503	79.640	1.00	21.98	C
	ATOM	936	O	PHE G 277	48.088	-24.707	80.395	1.00	21.74	O
	ATOM	937	CB	PHE G 277	46.714	-27.258	81.202	1.00	20.81	C
	ATOM	938	CG	PHE G 277	45.567	-27.891	81.933	1.00	19.89	C
	ATOM	939	CD1	PHE G 277	45.015	-29.081	81.490	1.00	19.94	C
	ATOM	940	CD2	PHE G 277	45.059	-27.312	83.092	1.00	21.02	C
	ATOM	941	CE1	PHE G 277	43.974	-29.697	82.190	1.00	20.42	C
	ATOM	942	CE2	PHE G 277	44.013	-27.921	83.800	1.00	21.46	C
	ATOM	943	CZ	PHE G 277	43.474	-29.118	83.347	1.00	20.53	C
	ATOM	944	N	THR G 278	47.962	-25.760	78.404	1.00	22.61	N
	ATOM	945	CA	THR G 278	49.139	-25.110	77.829	1.00	23.71	C
	ATOM	946	C	THR G 278	48.835	-23.739	77.203	1.00	23.69	C
	ATOM	947	O	THR G 278	49.607	-22.787	77.355	1.00	22.77	O
	ATOM	948	CB	THR G 278	49.787	-26.001	76.748	1.00	26.18	C
	ATOM	949	OG1	THR G 278	49.862	-27.355	77.218	1.00	29.00	O
	ATOM	950	CG2	THR G 278	51.200	-25.505	76.428	1.00	28.03	C
	ATOM	951	N	ASP G 279	47.743	-23.665	76.449	1.00	23.78	N
	ATOM	952	CA	ASP G 279	47.338	-22.426	75.802	1.00	22.85	C
	ATOM	953	C	ASP G 279	46.767	-21.521	76.875	1.00	21.97	C
	ATOM	954	O	ASP G 279	45.656	-21.741	77.354	1.00	21.82	O
	ATOM	955	CB	ASP G 279	46.272	-22.710	74.736	1.00	25.27	C
	ATOM	956	CG	ASP G 279	45.708	-21.420	74.008	1.00	26.22	C

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FIG. 53-22	ATOM 958	OD2 ASP G 279	44.644	-21.532	73.433	1.00	24.54	O
	ATOM 959	N ASN G 280	47.531	-20.503	77.248	1.00	20.54	N
	ATOM 960	CA ASN G 280	47.116	-19.549	78.275	1.00	19.55	C
	ATOM 961	C ASN G 280	45.782	-18.855	77.989	1.00	19.43	C
	ATOM 962	O ASN G 280	45.151	-18.317	78.893	1.00	20.85	O
	ATOM 963	CB ASN G 280	48.206	-18.493	78.499	1.00	17.41	C
	ATOM 964	CG ASN G 280	48.596	-17.764	77.220	1.00	15.05	C
	ATOM 965	OD1 ASN G 280	47.840	-17.716	76.241	1.00	13.88	O
	ATOM 966	ND2 ASN G 280	49.792	-17.201	77.220	1.00	12.65	N
	ATOM 967	N ALA G 281	45.355	-18.864	76.734	1.00	18.58	N
	ATOM 968	CA ALA G 281	44.107	-18.223	76.349	1.00	16.85	C
	ATOM 969	C ALA G 281	42.863	-18.972	76.786	1.00	16.69	C
	ATOM 970	O ALA G 281	41.784	-18.389	76.828	1.00	17.95	O
	ATOM 971	CB ALA G 281	44.072	-18.023	74.853	1.00	15.93	C
	ATOM 972	N LYS G 282	43.012	-20.248	77.135	1.00	16.80	N
	ATOM 973	CA LYS G 282	41.873	-21.081	77.517	1.00	14.67	C
	ATOM 974	C LYS G 282	41.472	-21.113	78.988	1.00	11.17	C
	ATOM 975	O LYS G 282	42.295	-21.293	79.875	1.00	8.39	O
	ATOM 976	CB LYS G 282	42.063	-22.499	76.973	1.00	17.48	C
	ATOM 977	CG LYS G 282	42.154	-22.568	75.439	1.00	21.17	C
	ATOM 978	CD LYS G 282	42.219	-24.024	74.973	1.00	24.20	C
	ATOM 979	CE LYS G 282	42.395	-24.173	73.455	1.00	23.38	C
	ATOM 980	NZ LYS G 282	43.820	-24.133	72.979	1.00	20.23	N
	ATOM 981	N THR G 283	40.177	-20.940	79.223	1.00	11.06	N
	ATOM 982	CA THR G 283	39.601	-20.935	80.561	1.00	10.51	C
	ATOM 983	C THR G 283	39.925	-22.237	81.297	1.00	11.20	C
	ATOM 984	O THR G 283	40.004	-23.309	80.692	1.00	12.03	O
	ATOM 985	CB THR G 283	38.049	-20.741	80.486	1.00	10.15	C
	ATOM 986	OG1 THR G 283	37.750	-19.505	79.819	1.00	10.23	O
	ATOM 987	CG2 THR G 283	37.419	-20.721	81.888	1.00	9.53	C
	ATOM 988	N ILE G 284	40.163	-22.119	82.595	1.00	11.90	N
	ATOM 989	CA ILE G 284	40.464	-23.263	83.449	1.00	11.48	C
	ATOM 990	C ILE G 284	39.347	-23.214	84.472	1.00	10.31	C
	ATOM 991	O ILE G 284	39.146	-22.186	85.112	1.00	9.75	O
	ATOM 992	CB ILE G 284	41.836	-23.096	84.173	1.00	11.66	C
	ATOM 993	CG1 ILE G 284	42.954	-22.932	83.146	1.00	11.57	C
	ATOM 994	CG2 ILE G 284	42.148	-24.313	85.042	1.00	10.67	C
	ATOM 995	CD1 ILE G 284	44.301	-22.643	83.766	1.00	11.86	C
	ATOM 996	N ILE G 285	38.547	-24.269	84.535	1.00	10.47	N
	ATOM 997	CA ILE G 285	37.439	-24.326	85.480	1.00	9.39	C
	ATOM 998	C ILE G 285	37.945	-25.046	86.718	1.00	10.51	C
	ATOM 999	O ILE G 285	38.764	-25.961	86.614	1.00	12.99	O
	ATOM 1000	CB ILE G 285	36.221	-25.084	84.892	1.00	8.03	C
	ATOM 1001	CG1 ILE G 285	35.891	-24.542	83.499	1.00	6.86	C
	ATOM 1002	CG2 ILE G 285	35.002	-24.894	85.785	1.00	7.78	C
	ATOM 1003	CD1 ILE G 285	34.648	-25.135	82.869	1.00	6.29	C
	ATOM 1004	N VAL G 286	37.466	-24.636	87.886	1.00	9.48	N
	ATOM 1005	CA VAL G 286	37.891	-25.237	89.140	1.00	6.38	C
	ATOM 1006	C VAL G 286	36.680	-25.691	89.931	1.00	6.91	C
	ATOM 1007	O VAL G 286	35.757	-24.914	90.182	1.00	6.45	O
	ATOM 1008	CB VAL G 286	38.693	-24.218	90.006	1.00	6.91	C
	ATOM 1009	CG1 VAL G 286	39.106	-24.842	91.336	1.00	3.92	C
	ATOM 1010	CG2 VAL G 286	39.914	-23.692	89.239	1.00	2.85	C
	ATOM 1011	N GLN G 287	36.679	-26.962	90.307	1.00	7.38	N
	ATOM 1012	CA GLN G 287	35.597	-27.526	91.089	1.00	8.03	C
	ATOM 1013	C GLN G 287	36.155	-27.618	92.489	1.00	10.75	C
	ATOM 1014	O GLN G 287	37.217	-28.224	92.719	1.00	11.57	O
	ATOM 1015	CB GLN G 287	35.194	-28.904	90.581	1.00	6.90	C
	ATOM 1016	CG GLN G 287	34.006	-29.480	91.322	1.00	6.23	C
	ATOM 1017	CD GLN G 287	33.402	-30.680	90.630	1.00	5.11	C
	ATOM 1018	OE1 GLN G 287	32.215	-30.695	90.337	1.00	7.55	O
	ATOM 1019	NE2 GLN G 287	34.216	-31.688	90.358	1.00	4.45	N
	ATOM 1020	N LEU G 288	35.457	-26.980	93.419	1.00	12.14	N
	ATOM 1021	CA LEU G 288	35.897	-26.930	94.797	1.00	13.73	C
	ATOM 1022	C LEU G 288	35.544	-28.111	95.679	1.00	16.56	C
	ATOM 1023	O LEU G 288	34.570	-28.830	95.440	1.00	18.23	O
	ATOM 1024	CB LEU G 288	35.395	-25.644	95.440	1.00	12.23	C
	ATOM 1025	CG LEU G 288	36.070	-24.354	94.998	1.00	8.03	C
	ATOM 1026	CD1 LEU G 288	35.785	-23.327	96.069	1.00	6.97	C
	ATOM 1027	CD2 LEU G 288	37.572	-24.551	94.868	1.00	5.62	C

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FIG. 53-23	ATOM 1029	CA ASN G 289	36.137 -29.343 97.697 1.00 22.89	C
	ATOM 1030	C ASN G 289	34.975 -29.000 98.617 1.00 24.07	C
	ATOM 1031	O ASN G 289	34.020 -29.768 98.749 1.00 24.32	O
	ATOM 1032	CB ASN G 289	37.390 -29.488 98.558 1.00 25.83	C
	ATOM 1033	CG ASN G 289	38.022 -30.841 98.432 1.00 29.22	C
	ATOM 1034	OD1 ASN G 289	37.414 -31.762 97.894 1.00 30.49	O
	ATOM 1035	ND2 ASN G 289	39.277 -30.942 98.875 1.00 32.39	N
	ATOM 1036	N THR G 290	35.064 -27.825 99.238 1.00 24.60	N
	ATOM 1037	CA THR G 290	34.057 -27.352 100.182 1.00 24.63	C
	ATOM 1038	C THR G 290	33.472 -26.014 99.721 1.00 23.12	C
	ATOM 1039	O THR G 290	34.164 -25.199 99.108 1.00 22.54	O
	ATOM 1040	CB THR G 290	34.688 -27.160 101.596 1.00 27.09	C
	ATOM 1041	OG1 THR G 290	35.516 -28.287 101.916 1.00 28.17	O
	ATOM 1042	CG2 THR G 290	33.600 -27.015 102.673 1.00 28.86	C
	ATOM 1043	N SER G 291	32.191 -25.805 100.011 1.00 22.35	N
	ATOM 1044	CA SER G 291	31.514 -24.564 99.655 1.00 21.82	C
	ATOM 1045	C SER G 291	32.006 -23.411 100.523 1.00 22.98	C
	ATOM 1046	O SER G 291	32.458 -23.603 101.661 1.00 22.87	O
	ATOM 1047	CB SER G 291	29.998 -24.697 99.825 1.00 20.36	C
	ATOM 1048	OG SER G 291	29.433 -25.549 98.847 1.00 19.98	O
	ATOM 1049	N VAL G 292	31.919 -22.212 99.965 1.00 23.56	N
	ATOM 1050	CA VAL G 292	32.323 -20.998 100.648 1.00 23.95	C
	ATOM 1051	C VAL G 292	31.083 -20.136 100.522 1.00 24.36	C
	ATOM 1052	O VAL G 292	30.268 -20.344 99.627 1.00 24.28	O
	ATOM 1053	CB VAL G 292	33.497 -20.292 99.940 1.00 24.28	C
	ATOM 1054	CG1 VAL G 292	34.110 -19.254 100.862 1.00 24.70	C
	ATOM 1055	CG2 VAL G 292	34.539 -21.297 99.484 1.00 24.60	C
	ATOM 1056	N GLU G 293	30.918 -19.185 101.424 1.00 24.79	N
	ATOM 1057	CA GLU G 293	29.746 -18.335 101.378 1.00 25.81	C
	ATOM 1058	C GLU G 293	30.106 -16.917 101.012 1.00 24.98	C
	ATOM 1059	O GLU G 293	31.195 -16.426 101.335 1.00 26.72	O
	ATOM 1060	CB GLU G 293	29.007 -18.372 102.718 1.00 26.15	C
	ATOM 1061	CG GLU G 293	28.460 -19.745 103.042 1.00 27.81	C
	ATOM 1062	CD GLU G 293	28.252 -19.948 104.512 1.00 29.06	C
	ATOM 1063	OE1 GLU G 293	29.244 -19.838 105.263 1.00 30.50	O
	ATOM 1064	OE2 GLU G 293	27.105 -20.234 104.920 1.00 31.07	O
	ATOM 1065	N ILE G 294	29.193 -16.292 100.291 1.00 22.44	N
	ATOM 1066	CA ILE G 294	29.343 -14.925 99.864 1.00 21.47	C
	ATOM 1067	C ILE G 294	27.973 -14.292 100.076 1.00 22.05	C
	ATOM 1068	O ILE G 294	26.999 -14.619 99.382 1.00 20.65	O
	ATOM 1069	CB ILE G 294	29.841 -14.830 98.393 1.00 19.43	C
	ATOM 1070	CG1 ILE G 294	29.820 -13.382 97.910 1.00 14.54	C
	ATOM 1071	CG2 ILE G 294	29.041 -15.747 97.480 1.00 21.41	C
	ATOM 1072	CD1 ILE G 294	30.557 -13.184 96.630 1.00 7.75	C
	ATOM 1073	N ASN G 295	27.890 -13.500 101.140 1.00 22.66	N
	ATOM 1074	CA ASN G 295	26.663 -12.806 101.512 1.00 23.48	C
	ATOM 1075	C ASN G 295	26.760 -11.408 100.912 1.00 22.67	C
	ATOM 1076	O ASN G 295	27.787 -10.733 101.048 1.00 21.79	O
	ATOM 1077	CB ASN G 295	26.526 -12.744 103.044 1.00 26.38	C
	ATOM 1078	CG ASN G 295	26.744 -14.104 103.712 1.00 30.07	C
	ATOM 1079	OD1 ASN G 295	27.501 -14.929 103.197 1.00 31.57	O
	ATOM 1080	ND2 ASN G 295	26.102 -14.347 104.854 1.00 32.72	N
	ATOM 1081	N CYS G 296	25.711 -10.999 100.205 1.00 23.39	N
	ATOM 1082	CA CYS G 296	25.680 -9.693 99.555 1.00 23.29	C
	ATOM 1083	C CYS G 296	24.345 -8.990 99.773 1.00 22.56	C
	ATOM 1084	O CYS G 296	23.324 -9.641 100.001 1.00 20.72	O
	ATOM 1085	CB CYS G 296	25.890 -9.853 98.049 1.00 24.78	C
	ATOM 1086	SG CYS G 296	27.397 -10.728 97.530 1.00 27.71	S
	ATOM 1087	N THR G 297	24.367 -7.665 99.647 1.00 22.54	N
	ATOM 1088	CA THR G 297	23.188 -6.819 99.791 1.00 23.05	C
	ATOM 1089	C THR G 297	23.247 -5.695 98.767 1.00 22.63	C
	ATOM 1090	O THR G 297	24.331 -5.333 98.301 1.00 22.80	O
	ATOM 1091	CB THR G 297	23.123 -6.169 101.178 1.00 24.92	C
	ATOM 1092	OG1 THR G 297	24.453 -5.961 101.665 1.00 27.02	O
	ATOM 1093	CG2 THR G 297	22.336 -7.023 102.147 1.00 25.66	C
	ATOM 1094	N GLY G 298	22.091 -5.109 98.461 1.00 22.54	N
	ATOM 1095	CA GLY G 298	22.029 -4.012 97.504 1.00 22.48	C
	ATOM 1096	C GLY G 298	22.834 -2.795 97.940 1.00 21.63	C
	ATOM 1097	O GLY G 298	23.237 -1.978 97.110 1.00 22.39	O
	ATOM 1098	N ALA G 299	23.107 -2.716 99.242 1.00 20.04	N



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FIG. 53-24	ATOM 1100 C ALA G 299	25.329	-1.540	99.408	1.00	18.55	C
	ATOM 1101 O ALA G 299	26.147	-0.898	100.061	1.00	17.42	O
	ATOM 1102 CB ALA G 299	23.822	-1.781	101.381	1.00	18.00	C
	ATOM 1103 N GLY G 329	25.671	-2.248	98.340	1.00	20.79	N
	ATOM 1104 CA GLY G 329	27.013	-2.165	97.804	1.00	21.75	C
	ATOM 1105 C GLY G 329	28.117	-3.093	98.261	1.00	21.66	C
	ATOM 1106 O GLY G 329	29.258	-2.900	97.858	1.00	21.50	O
	ATOM 1107 N HIS G 330	27.835	-4.105	99.070	1.00	22.43	N
	ATOM 1108 CA HIS G 330	28.926	-4.983	99.481	1.00	22.31	C
	ATOM 1109 C HIS G 330	28.617	-6.461	99.535	1.00	21.45	C
	ATOM 1110 O HIS G 330	27.458	-6.883	99.533	1.00	19.33	O
	ATOM 1111 CB HIS G 330	29.563	-4.532	100.801	1.00	23.24	C
	ATOM 1112 CG HIS G 330	28.574	-4.278	101.892	1.00	27.00	C
	ATOM 1113 ND1 HIS G 330	27.850	-5.258	102.527	1.00	27.17	N
	ATOM 1114 CD2 HIS G 330	28.168	-3.105	102.443	1.00	28.95	C
	ATOM 1115 CE1 HIS G 330	27.044	-4.667	103.417	1.00	28.28	C
	ATOM 1116 NE2 HIS G 330	27.204	-3.360	103.401	1.00	29.66	N
	ATOM 1117 N CYS G 331	29.696	-7.233	99.510	1.00	22.55	N
	ATOM 1118 CA CYS G 331	29.657	-8.682	99.575	1.00	24.15	C
	ATOM 1119 C CYS G 331	30.739	-9.099	100.541	1.00	24.13	C
	ATOM 1120 O CYS G 331	31.898	-8.726	100.370	1.00	24.27	O
	ATOM 1121 CB CYS G 331	29.986	-9.299	98.220	1.00	24.97	C
	ATOM 1122 SG CYS G 331	28.657	-9.223	97.000	1.00	28.48	S
	ATOM 1123 N ASN G 332	30.382	-9.822	101.588	1.00	24.96	N
	ATOM 1124 CA ASN G 332	31.425	-10.249	102.490	1.00	26.49	C
	ATOM 1125 C ASN G 332	31.491	-11.767	102.519	1.00	24.08	C
	ATOM 1126 O ASN G 332	30.474	-12.459	102.448	1.00	21.19	O
	ATOM 1127 CB ASN G 332	31.289	-9.616	103.885	1.00	31.67	C
	ATOM 1128 CG ASN G 332	30.507	-10.472	104.852	1.00	38.18	C
	ATOM 1129 OD1 ASN G 332	31.086	-11.014	105.792	1.00	41.31	O
	ATOM 1130 ND2 ASN G 332	29.213	-10.640	104.604	1.00	41.97	N
	ATOM 1131 N ILE G 333	32.716	-12.258	102.470	1.00	23.04	N
	ATOM 1132 CA ILE G 333	33.005	-13.677	102.489	1.00	23.16	C
	ATOM 1133 C ILE G 333	34.098	-13.916	103.544	1.00	23.36	C
	ATOM 1134 O ILE G 333	35.029	-13.109	103.685	1.00	21.86	O
	ATOM 1135 CB ILE G 333	33.422	-14.178	101.062	1.00	21.56	C
	ATOM 1136 CG1 ILE G 333	34.577	-15.170	101.137	1.00	19.40	C
	ATOM 1137 CG2 ILE G 333	33.748	-12.997	100.141	1.00	22.44	C
	ATOM 1138 CD1 ILE G 333	35.100	-15.539	99.807	1.00	17.23	C
	ATOM 1139 N SER G 334	33.953	-14.992	104.315	1.00	22.28	N
	ATOM 1140 CA SER G 334	34.917	-15.324	105.355	1.00	22.05	C
	ATOM 1141 C SER G 334	36.355	-15.342	104.839	1.00	22.63	C
	ATOM 1142 O SER G 334	36.673	-15.995	103.847	1.00	22.64	O
	ATOM 1143 CB SER G 334	34.560	-16.662	105.997	1.00	22.04	C
	ATOM 1144 OG SER G 334	33.172	-16.722	106.305	1.00	22.98	O
	ATOM 1145 N ARG G 335	37.207	-14.589	105.516	1.00	24.33	N
	ATOM 1146 CA ARG G 335	38.617	-14.473	105.174	1.00	26.14	C
	ATOM 1147 C ARG G 335	39.384	-15.794	105.297	1.00	26.30	C
	ATOM 1148 O ARG G 335	40.233	-16.103	104.464	1.00	26.93	O
	ATOM 1149 CB ARG G 335	39.246	-13.419	106.085	1.00	28.38	C
	ATOM 1150 CG ARG G 335	40.747	-13.345	106.044	1.00	32.38	C
	ATOM 1151 CD ARG G 335	41.256	-12.299	107.027	1.00	39.28	C
	ATOM 1152 NE ARG G 335	40.577	-11.012	106.869	1.00	44.47	N
	ATOM 1153 CZ ARG G 335	40.903	-9.902	107.526	1.00	48.65	C
	ATOM 1154 NH1 ARG G 335	41.915	-9.906	108.386	1.00	50.25	N
	ATOM 1155 NH2 ARG G 335	40.184	-8.799	107.363	1.00	50.93	N
	ATOM 1156 N ALA G 336	39.105	-16.549	106.358	1.00	25.12	N
	ATOM 1157 CA ALA G 336	39.777	-17.820	106.603	1.00	23.00	C
	ATOM 1158 C ALA G 336	39.305	-18.899	105.634	1.00	22.42	C
	ATOM 1159 O ALA G 336	40.128	-19.554	104.981	1.00	21.64	O
	ATOM 1160 CB ALA G 336	39.563	-18.259	108.034	1.00	23.10	C
	ATOM 1161 N LYS G 337	37.985	-19.048	105.507	1.00	21.05	N
	ATOM 1162 CA LYS G 337	37.405	-20.040	104.608	1.00	20.30	C
	ATOM 1163 C LYS G 337	37.964	-19.926	103.202	1.00	20.37	C
	ATOM 1164 O LYS G 337	38.345	-20.926	102.597	1.00	20.21	O
	ATOM 1165 CB LYS G 337	35.886	-19.907	104.540	1.00	20.28	C
	ATOM 1166 CG LYS G 337	35.121	-20.622	105.642	1.00	22.99	C
	ATOM 1167 CD LYS G 337	33.606	-20.410	105.465	1.00	25.82	C
	ATOM 1168 CE LYS G 337	32.784	-20.963	106.637	1.00	26.21	C
	ATOM 1169 N7 LYS G 337	31.477	-20.343	106.712	1.00	27.47	N

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FIG. 53-25	ATOM 1171 CA TRP G 338	38.528 -18.528 101.324 1.00 21.84	C
	ATOM 1172 C TRP G 338	40.036 -18.605 101.126 1.00 22.14	C
	ATOM 1173 O TRP G 338	40.498 -18.997 100.050 1.00 21.87	O
	ATOM 1174 CB TRP G 338	37.983 -17.238 100.704 1.00 20.93	C
	ATOM 1175 CG TRP G 338	37.657 -17.425 99.263 1.00 20.83	C
	ATOM 1176 CD1 TRP G 338	36.578 -18.083 98.743 1.00 22.75	C
	ATOM 1177 CD2 TRP G 338	38.426 -16.979 98.144 1.00 19.66	C
	ATOM 1178 NE1 TRP G 338	36.627 -18.071 97.368 1.00 22.40	N
	ATOM 1179 CE2 TRP G 338	37.753 -17.403 96.975 1.00 19.83	C
	ATOM 1180 CE3 TRP G 338	39.618 -16.261 98.012 1.00 19.32	C
	ATOM 1181 CZ2 TRP G 338	38.231 -17.134 95.696 1.00 21.02	C
	ATOM 1182 CZ3 TRP G 338	40.091 -15.997 96.743 1.00 21.47	C
	ATOM 1183 CH2 TRP G 338	39.400 -16.432 95.599 1.00 21.53	C
	ATOM 1184 N ASN G 339	40.812 -18.216 102.132 1.00 22.61	N
	ATOM 1185 CA ASN G 339	42.256 -18.276 101.969 1.00 25.09	C
	ATOM 1186 C ASN G 339	42.681 -19.747 101.917 1.00 24.55	C
	ATOM 1187 O ASN G 339	43.653 -20.109 101.250 1.00 23.39	O
	ATOM 1188 CB ASN G 339	42.972 -17.521 103.090 1.00 29.69	C
	ATOM 1189 CG ASN G 339	44.411 -17.175 102.733 1.00 37.25	C
	ATOM 1190 OD1 ASN G 339	45.358 -17.669 103.354 1.00 38.36	O
	ATOM 1191 ND2 ASN G 339	44.579 -16.334 101.712 1.00 44.12	N
	ATOM 1192 N ASN G 340	41.898 -20.597 102.574 1.00 24.15	N
	ATOM 1193 CA ASN G 340	42.162 -22.028 102.602 1.00 24.49	C
	ATOM 1194 C ASN G 340	41.929 -22.666 101.228 1.00 22.71	C
	ATOM 1195 O ASN G 340	42.763 -23.431 100.742 1.00 22.28	O
	ATOM 1196 CB ASN G 340	41.285 -22.715 103.652 1.00 28.25	C
	ATOM 1197 CG ASN G 340	41.691 -24.158 103.901 1.00 32.25	C
	ATOM 1198 OD1 ASN G 340	41.044 -25.090 103.421 1.00 34.35	O
	ATOM 1199 ND2 ASN G 340	42.776 -24.348 104.646 1.00 32.79	N
	ATOM 1200 N THR G 341	40.804 -22.344 100.595 1.00 20.42	N
	ATOM 1201 CA THR G 341	40.498 -22.898 99.275 1.00 18.47	C
	ATOM 1202 C THR G 341	41.539 -22.452 98.256 1.00 16.79	C
	ATOM 1203 O THR G 341	41.774 -23.132 97.253 1.00 16.74	O
	ATOM 1204 CB THR G 341	39.106 -22.458 98.758 1.00 18.47	C
	ATOM 1205 OG1 THR G 341	39.154 -21.093 98.322 1.00 15.57	O
	ATOM 1206 CG2 THR G 341	38.063 -22.601 99.857 1.00 17.91	C
	ATOM 1207 N LEU G 342	42.160 -21.306 98.515 1.00 15.68	N
	ATOM 1208 CA LEU G 342	43.162 -20.765 97.614 1.00 15.72	C
	ATOM 1209 C LEU G 342	44.400 -21.624 97.584 1.00 15.53	C
	ATOM 1210 O LEU G 342	44.904 -21.940 96.510 1.00 15.44	O
	ATOM 1211 CB LEU G 342	43.521 -19.332 98.000 1.00 18.54	C
	ATOM 1212 CG LEU G 342	42.615 -18.175 97.567 1.00 18.13	C
	ATOM 1213 CD1 LEU G 342	42.933 -16.964 98.423 1.00 15.23	C
	ATOM 1214 CD2 LEU G 342	42.794 -17.866 96.079 1.00 14.33	C
	ATOM 1215 N LYS G 343	44.882 -22.027 98.758 1.00 16.83	N
	ATOM 1216 CA LYS G 343	46.077 -22.869 98.825 1.00 17.44	C
	ATOM 1217 C LYS G 343	45.775 -24.266 98.306 1.00 18.33	C
	ATOM 1218 O LYS G 343	46.680 -24.992 97.920 1.00 19.02	O
	ATOM 1219 CB LYS G 343	46.672 -22.924 100.238 1.00 15.61	C
	ATOM 1220 CG LYS G 343	45.875 -23.699 101.266 1.00 17.55	C
	ATOM 1221 CD LYS G 343	46.755 -24.097 102.450 1.00 19.36	C
	ATOM 1222 CE LYS G 343	47.847 -25.094 102.038 1.00 22.94	C
	ATOM 1223 NZ LYS G 343	47.289 -26.365 101.448 1.00 25.97	N
	ATOM 1224 N GLN G 344	44.503 -24.651 98.334 1.00 19.88	N
	ATOM 1225 CA GLN G 344	44.084 -25.948 97.820 1.00 22.64	C
	ATOM 1226 C GLN G 344	44.181 -25.876 96.294 1.00 24.58	C
	ATOM 1227 O GLN G 344	44.821 -26.719 95.661 1.00 27.10	O
	ATOM 1228 CB GLN G 344	42.648 -26.269 98.237 1.00 22.13	C
	ATOM 1229 CG GLN G 344	42.470 -26.496 99.728 1.00 23.77	C
	ATOM 1230 CD GLN G 344	41.046 -26.867 100.099 1.00 25.77	C
	ATOM 1231 OE1 GLN G 344	40.126 -26.805 99.270 1.00 29.28	O
	ATOM 1232 NE2 GLN G 344	40.853 -27.257 101.349 1.00 25.33	N
	ATOM 1233 N ILE G 345	43.565 -24.849 95.713 1.00 24.68	N
	ATOM 1234 CA ILE G 345	43.601 -24.645 94.274 1.00 23.26	C
	ATOM 1235 C ILE G 345	45.057 -24.451 93.871 1.00 22.65	C
	ATOM 1236 O ILE G 345	45.463 -24.877 92.791 1.00 24.30	O
	ATOM 1237 CB ILE G 345	42.803 -23.386 93.861 1.00 24.27	C
	ATOM 1238 CG1 ILE G 345	41.344 -23.508 94.325 1.00 23.39	C
	ATOM 1239 CG2 ILE G 345	42.894 -23.172 92.347 1.00 22.15	C
	ATOM 1240 CD1 ILE G 345	40.500 -22.777 94.070 1.00 20.40	C

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FIG. 53-26

ATOM 1242	CA ALA G 346	47.261	-23.598	94.462	1.00	19.48	C
ATOM 1243	C ALA G 346	48.045	-24.906	94.412	1.00	20.48	C
ATOM 1244	O ALA G 346	49.036	-25.020	93.697	1.00	20.51	O
ATOM 1245	CB ALA G 346	47.859	-22.658	95.501	1.00	17.62	C
ATOM 1246	N SER G 347	47.553	-25.911	95.126	1.00	22.28	N
ATOM 1247	CA SER G 347	48.199	-27.212	95.169	1.00	24.38	C
ATOM 1248	C SER G 347	47.989	-28.031	93.901	1.00	26.23	C
ATOM 1249	O SER G 347	47.940	-29.261	93.966	1.00	26.76	O
ATOM 1250	CB SER G 347	47.699	-28.008	96.375	1.00	24.17	C
ATOM 1251	OG SER G 347	48.063	-27.385	97.598	1.00	24.21	O
ATOM 1252	N LYS G 348	47.839	-27.364	92.757	1.00	29.96	N
ATOM 1253	CA LYS G 348	47.642	-28.065	91.489	1.00	33.03	C
ATOM 1254	C LYS G 348	47.559	-27.230	90.221	1.00	35.63	C
ATOM 1255	O LYS G 348	47.321	-27.788	89.152	1.00	38.39	O
ATOM 1256	CB LYS G 348	46.413	-28.975	91.565	1.00	32.95	C
ATOM 1257	CG LYS G 348	45.129	-28.281	91.999	1.00	33.51	C
ATOM 1258	CD LYS G 348	44.028	-29.304	92.276	1.00	31.97	C
ATOM 1259	CE LYS G 348	43.720	-30.135	91.034	1.00	30.77	C
ATOM 1260	NZ LYS G 348	43.968	-31.571	91.245	1.00	29.18	N
ATOM 1261	N LEU G 349	47.844	-25.935	90.296	1.00	37.19	N
ATOM 1262	CA LEU G 349	47.740	-25.060	89.121	1.00	39.86	C
ATOM 1263	C LEU G 349	48.595	-25.380	87.879	1.00	40.94	C
ATOM 1264	O LEU G 349	49.636	-26.019	87.995	1.00	40.31	O
ATOM 1265	CB LEU G 349	47.868	-23.602	89.553	1.00	39.82	C
ATOM 1266	CG LEU G 349	46.582	-23.193	90.277	1.00	39.38	C
ATOM 1267	CD1 LEU G 349	46.704	-21.816	90.896	1.00	38.81	C
ATOM 1268	CD2 LEU G 349	45.419	-23.268	89.287	1.00	38.70	C
ATOM 1269	N ARG G 350	48.123	-24.926	86.708	1.00	42.25	N
ATOM 1270	CA ARG G 350	48.719	-25.151	85.371	1.00	42.80	C
ATOM 1271	C ARG G 350	49.867	-26.116	85.187	1.00	43.82	C
ATOM 1272	O ARG G 350	49.823	-26.941	84.275	1.00	45.61	O
ATOM 1273	CB ARG G 350	49.039	-23.866	84.619	1.00	43.22	C
ATOM 1274	CG ARG G 350	49.218	-24.105	83.101	1.00	45.68	C
ATOM 1275	CD ARG G 350	50.614	-24.613	82.682	1.00	49.73	C
ATOM 1276	NE ARG G 350	50.589	-25.386	81.431	1.00	52.41	N
ATOM 1277	CZ ARG G 350	51.606	-26.114	80.961	1.00	51.60	C
ATOM 1278	NH1 ARG G 350	52.750	-26.185	81.632	1.00	53.56	N
ATOM 1279	NH2 ARG G 350	51.476	-26.793	79.831	1.00	51.64	N
ATOM 1280	N GLU G 351	50.932	-25.965	85.967	1.00	43.58	N
ATOM 1281	CA GLU G 351	52.082	-26.872	85.906	1.00	43.20	C
ATOM 1282	C GLU G 351	51.500	-28.298	85.840	1.00	43.33	C
ATOM 1283	O GLU G 351	52.113	-29.209	85.285	1.00	42.89	O
ATOM 1284	CB GLU G 351	52.924	-26.670	87.174	1.00	43.52	C
ATOM 1285	CG GLU G 351	54.310	-27.289	87.200	1.00	41.21	C
ATOM 1286	CD GLU G 351	55.019	-27.057	88.534	1.00	41.51	C
ATOM 1287	OE1 GLU G 351	54.342	-26.751	89.541	1.00	40.87	O
ATOM 1288	OE2 GLU G 351	56.259	-27.169	88.583	1.00	42.54	O
ATOM 1289	N GLN G 352	50.280	-28.429	86.375	1.00	43.75	N
ATOM 1290	CA GLN G 352	49.473	-29.647	86.408	1.00	45.18	C
ATOM 1291	C GLN G 352	49.718	-30.460	87.656	1.00	46.24	C
ATOM 1292	O GLN G 352	50.300	-31.549	87.611	1.00	46.13	O
ATOM 1293	CB GLN G 352	49.649	-30.483	85.132	1.00	45.24	C
ATOM 1294	CG GLN G 352	48.880	-29.946	83.930	1.00	43.09	C
ATOM 1295	CD GLN G 352	47.404	-29.785	84.226	1.00	42.64	C
ATOM 1296	OE1 GLN G 352	46.589	-30.619	83.838	1.00	42.75	O
ATOM 1297	NE2 GLN G 352	47.051	-28.708	84.922	1.00	41.31	N
ATOM 1298	N PHE G 353	49.221	-29.927	88.770	1.00	47.62	N
ATOM 1299	CA PHE G 353	49.396	-30.535	90.086	1.00	49.37	C
ATOM 1300	C PHE G 353	50.909	-30.583	90.244	1.00	50.92	C
ATOM 1301	O PHE G 353	51.465	-31.458	90.910	1.00	51.55	O
ATOM 1302	CB PHE G 353	48.784	-31.939	90.124	1.00	48.39	C
ATOM 1303	CG PHE G 353	48.379	-32.391	91.499	1.00	47.75	C
ATOM 1304	CD1 PHE G 353	49.304	-32.437	92.536	1.00	47.81	C
ATOM 1305	CD2 PHE G 353	47.071	-32.794	91.750	1.00	47.05	C
ATOM 1306	CE1 PHE G 353	48.936	-32.876	93.804	1.00	48.78	C
ATOM 1307	CE2 PHE G 353	46.691	-33.234	93.013	1.00	47.45	C
ATOM 1308	CZ PHE G 353	47.625	-33.276	94.042	1.00	48.43	C
ATOM 1309	N GLY G 354	51.556	-29.613	89.602	1.00	52.21	N
ATOM 1310	CA GLY G 354	52.996	-29.519	89.600	1.00	55.31	C
ATOM 1311	C GLY G 354	53.673	-30.810	90.936	1.00	57.00	C

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FIG. 53-27

ATOM 1313	N ASN G 355	54.716	-30.563	90.895	1.00	56.63	N
ATOM 1314	CA ASN G 355	55.437	-30.927	92.100	1.00	55.92	C
ATOM 1315	C ASN G 355	55.702	-29.673	92.922	1.00	54.78	C
ATOM 1316	O ASN G 355	55.635	-29.727	94.155	1.00	55.56	O
ATOM 1317	CB ASN G 355	56.729	-31.658	91.742	1.00	56.52	C
ATOM 1318	CG ASN G 355	56.474	-32.950	90.982	1.00	57.60	C
ATOM 1319	OD1 ASN G 355	57.404	-33.565	90.467	1.00	60.33	O
ATOM 1320	ND2 ASN G 355	55.212	-33.359	90.895	1.00	56.65	N
ATOM 1321	N ASN G 356	55.994	-28.560	92.238	1.00	51.48	N
ATOM 1322	CA ASN G 356	56.209	-27.270	92.891	1.00	48.76	C
ATOM 1323	C ASN G 356	56.815	-26.133	92.083	1.00	47.04	C
ATOM 1324	O ASN G 356	57.690	-26.330	91.233	1.00	46.83	O
ATOM 1325	CB ASN G 356	56.969	-27.398	94.205	1.00	49.07	C
ATOM 1326	CG ASN G 356	56.270	-26.671	95.331	1.00	50.28	C
ATOM 1327	OD1 ASN G 356	55.666	-25.613	95.121	1.00	49.32	O
ATOM 1328	ND2 ASN G 356	56.322	-27.241	96.528	1.00	50.39	N
ATOM 1329	N LYS G 357	56.344	-24.932	92.417	1.00	44.39	N
ATOM 1330	CA LYS G 357	56.759	-23.666	91.824	1.00	41.03	C
ATOM 1331	C LYS G 357	55.913	-22.592	92.496	1.00	40.06	C
ATOM 1332	O LYS G 357	55.035	-22.899	93.307	1.00	40.50	O
ATOM 1333	CB LYS G 357	56.537	-23.631	90.316	1.00	39.41	C
ATOM 1334	CG LYS G 357	55.084	-23.571	89.867	1.00	37.01	C
ATOM 1335	CD LYS G 357	55.017	-23.221	88.392	1.00	35.55	C
ATOM 1336	CE LYS G 357	56.110	-23.954	87.642	1.00	33.79	C
ATOM 1337	NZ LYS G 357	56.188	-23.600	86.218	1.00	34.41	N
ATOM 1338	N THR G 358	56.160	-21.337	92.150	1.00	37.88	N
ATOM 1339	CA THR G 358	55.430	-20.231	92.746	1.00	35.21	C
ATOM 1340	C THR G 358	54.093	-20.001	92.042	1.00	32.30	C
ATOM 1341	O THR G 358	54.055	-19.800	90.826	1.00	32.63	O
ATOM 1342	CB THR G 358	56.270	-18.922	92.688	1.00	36.59	C
ATOM 1343	OG1 THR G 358	57.648	-19.203	92.988	1.00	36.43	O
ATOM 1344	CG2 THR G 358	55.738	-17.902	93.691	1.00	36.20	C
ATOM 1345	N ILE G 359	53.002	-20.066	92.798	1.00	28.71	N
ATOM 1346	CA ILE G 359	51.667	-19.833	92.255	1.00	25.73	C
ATOM 1347	C ILE G 359	51.187	-18.455	92.712	1.00	25.01	C
ATOM 1348	O ILE G 359	51.098	-18.175	93.910	1.00	25.59	O
ATOM 1349	CB ILE G 359	50.664	-20.923	92.700	1.00	25.07	C
ATOM 1350	CG1 ILE G 359	50.695	-22.099	91.723	1.00	23.68	C
ATOM 1351	CG2 ILE G 359	49.245	-20.367	92.786	1.00	24.79	C
ATOM 1352	CD1 ILE G 359	51.903	-22.969	91.841	1.00	24.61	C
ATOM 1353	N ILE G 360	50.859	-17.599	91.755	1.00	23.10	N
ATOM 1354	CA ILE G 360	50.423	-16.252	92.074	1.00	20.52	C
ATOM 1355	C ILE G 360	49.004	-15.969	91.600	1.00	21.12	C
ATOM 1356	O ILE G 360	48.611	-16.308	90.477	1.00	19.68	O
ATOM 1357	CB ILE G 360	51.386	-15.193	91.474	1.00	18.01	C
ATOM 1358	CG1 ILE G 360	52.818	-15.474	91.921	1.00	19.32	C
ATOM 1359	CG2 ILE G 360	51.009	-13.806	91.945	1.00	16.83	C
ATOM 1360	CD1 ILE G 360	53.863	-14.699	91.178	1.00	20.28	C
ATOM 1361	N PHE G 361	48.232	-15.375	92.498	1.00	21.60	N
ATOM 1362	CA PHE G 361	46.867	-14.990	92.223	1.00	20.51	C
ATOM 1363	C PHE G 361	46.838	-13.468	92.138	1.00	20.25	C
ATOM 1364	O PHE G 361	47.157	-12.789	93.115	1.00	20.96	O
ATOM 1365	CB PHE G 361	45.939	-15.457	93.348	1.00	18.51	C
ATOM 1366	CG PHE G 361	45.647	-16.935	93.330	1.00	19.11	C
ATOM 1367	CD1 PHE G 361	45.126	-17.546	92.191	1.00	19.66	C
ATOM 1368	CD2 PHE G 361	45.875	-17.718	94.458	1.00	17.60	C
ATOM 1369	CE1 PHE G 361	44.840	-18.915	92.181	1.00	18.26	C
ATOM 1370	CE2 PHE G 361	45.593	-19.080	94.450	1.00	16.64	C
ATOM 1371	CZ PHE G 361	45.075	-19.678	93.311	1.00	16.40	C
ATOM 1372	N LYS G 362	46.581	-12.951	90.940	1.00	19.16	N
ATOM 1373	CA LYS G 362	46.456	-11.512	90.707	1.00	17.16	C
ATOM 1374	C LYS G 362	45.026	-11.365	90.215	1.00	16.29	C
ATOM 1375	O LYS G 362	44.293	-12.353	90.132	1.00	16.31	O
ATOM 1376	CB LYS G 362	47.395	-11.011	89.603	1.00	16.96	C
ATOM 1377	CG LYS G 362	48.850	-10.842	89.992	1.00	17.71	C
ATOM 1378	CD LYS G 362	49.596	-10.118	88.874	1.00	18.34	C
ATOM 1379	CE LYS G 362	51.021	-10.631	88.709	1.00	17.10	C
ATOM 1380	NZ LYS G 362	51.864	-10.418	89.909	1.00	18.10	N
ATOM 1381	N GLN G 363	44.625	-10.149	89.861	1.00	15.68	N
ATOM 1382	CA GLN G 363	43.772	-9.048	89.777	1.00	15.77	C

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FIG. 53-28

ATOM 1384	O GLN G 363	44.245	-9.483	87.236	1.00	13.77	O
ATOM 1385	CB GLN G 363	42.529	-8.939	90.231	1.00	19.40	C
ATOM 1386	CG GLN G 363	41.196	-9.469	90.728	1.00	24.43	C
ATOM 1387	CD GLN G 363	40.033	-8.844	90.008	1.00	27.66	C
ATOM 1388	OE1 GLN G 363	39.942	-7.621	89.904	1.00	29.28	O
ATOM 1389	NE2 GLN G 363	39.123	-9.671	89.518	1.00	29.73	N
ATOM 1390	N SER G 364	41.996	-9.403	87.413	1.00	12.57	N
ATOM 1391	CA SER G 364	41.775	-9.117	86.016	1.00	12.09	C
ATOM 1392	C SER G 364	42.651	-8.048	85.392	1.00	14.93	C
ATOM 1393	O SER G 364	42.913	-7.004	85.994	1.00	15.10	O
ATOM 1394	CB SER G 364	40.317	-8.783	85.783	1.00	11.50	C
ATOM 1395	OG SER G 364	40.006	-8.944	84.414	1.00	12.57	O
ATOM 1396	N SER G 365	43.107	-8.333	84.174	1.00	16.70	N
ATOM 1397	CA SER G 365	43.941	-7.409	83.412	1.00	15.93	C
ATOM 1398	C SER G 365	43.067	-6.254	82.898	1.00	14.17	C
ATOM 1399	O SER G 365	43.514	-5.103	82.821	1.00	12.17	O
ATOM 1400	CB SER G 365	44.572	-8.129	82.220	1.00	15.75	C
ATOM 1401	OG SER G 365	45.334	-9.256	82.612	1.00	17.45	O
ATOM 1402	N GLY G 366	41.835	-6.581	82.515	1.00	11.39	N
ATOM 1403	CA GLY G 366	40.931	-5.571	82.002	1.00	9.59	C
ATOM 1404	C GLY G 366	39.815	-6.159	81.165	1.00	7.26	C
ATOM 1405	O GLY G 366	39.727	-7.377	81.003	1.00	5.86	O
ATOM 1406	N GLY G 367	38.993	-5.286	80.594	1.00	6.94	N
ATOM 1407	CA GLY G 367	37.877	-5.730	79.779	1.00	6.56	C
ATOM 1408	C GLY G 367	36.551	-5.336	80.396	1.00	6.41	C
ATOM 1409	O GLY G 367	36.512	-4.652	81.419	1.00	4.55	O
ATOM 1410	N ASP G 368	35.463	-5.785	79.782	1.00	8.86	N
ATOM 1411	CA ASP G 368	34.111	-5.480	80.254	1.00	11.00	C
ATOM 1412	C ASP G 368	33.917	-5.533	81.767	1.00	12.56	C
ATOM 1413	O ASP G 368	34.601	-6.284	82.470	1.00	14.21	O
ATOM 1414	CB ASP G 368	33.118	-6.431	79.603	1.00	11.95	C
ATOM 1415	CG ASP G 368	32.804	-6.052	78.182	1.00	14.99	C
ATOM 1416	OD1 ASP G 368	33.720	-5.637	77.432	1.00	15.86	O
ATOM 1417	OD2 ASP G 368	31.627	-6.185	77.800	1.00	14.92	O
ATOM 1418	N PRO G 369	32.957	-4.750	82.292	1.00	12.32	N
ATOM 1419	CA PRO G 369	32.703	-4.741	83.726	1.00	11.90	C
ATOM 1420	C PRO G 369	32.277	-6.132	84.202	1.00	11.43	C
ATOM 1421	O PRO G 369	32.726	-6.598	85.239	1.00	11.49	O
ATOM 1422	CB PRO G 369	31.562	-3.730	83.852	1.00	12.76	C
ATOM 1423	CG PRO G 369	31.783	-2.809	82.728	1.00	10.24	C
ATOM 1424	CD PRO G 369	32.084	-3.773	81.622	1.00	13.28	C
ATOM 1425	N GLU G 370	31.450	-6.807	83.410	1.00	11.25	N
ATOM 1426	CA GLU G 370	30.954	-8.149	83.747	1.00	11.17	C
ATOM 1427	C GLU G 370	32.078	-9.175	83.855	1.00	9.72	C
ATOM 1428	O GLU G 370	31.950	-10.168	84.563	1.00	9.84	O
ATOM 1429	CB GLU G 370	29.939	-8.628	82.709	1.00	12.14	C
ATOM 1430	CG GLU G 370	28.763	-7.683	82.449	1.00	14.26	C
ATOM 1431	CD GLU G 370	29.133	-6.422	81.665	1.00	13.73	C
ATOM 1432	OE1 GLU G 370	30.216	-6.377	81.046	1.00	15.24	O
ATOM 1433	OE2 GLU G 370	28.335	-5.463	81.652	1.00	12.38	O
ATOM 1434	N ILE G 371	33.171	-8.919	83.141	1.00	8.48	N
ATOM 1435	CA ILE G 371	34.359	-9.777	83.114	1.00	6.27	C
ATOM 1436	C ILE G 371	35.372	-9.461	84.213	1.00	5.63	C
ATOM 1437	O ILE G 371	35.946	-10.375	84.819	1.00	3.51	O
ATOM 1438	CB ILE G 371	35.057	-9.664	81.726	1.00	7.86	C
ATOM 1439	CG1 ILE G 371	34.249	-10.438	80.699	1.00	10.27	C
ATOM 1440	CG2 ILE G 371	36.518	-10.107	81.770	1.00	5.95	C
ATOM 1441	CD1 ILE G 371	33.646	-11.702	81.270	1.00	14.03	C
ATOM 1442	N VAL G 372	35.609	-8.163	84.420	1.00	5.08	N
ATOM 1443	CA VAL G 372	36.553	-7.638	85.406	1.00	5.14	C
ATOM 1444	C VAL G 372	36.064	-7.739	86.862	1.00	6.39	C
ATOM 1445	O VAL G 372	36.860	-7.658	87.808	1.00	4.88	O
ATOM 1446	CB VAL G 372	36.884	-6.163	85.084	1.00	4.04	C
ATOM 1447	CG1 VAL G 372	37.827	-5.577	86.108	1.00	4.81	C
ATOM 1448	CG2 VAL G 372	37.525	-6.075	83.734	1.00	5.30	C
ATOM 1449	N THR G 373	34.766	-7.939	87.046	1.00	7.07	N
ATOM 1450	CA THR G 373	34.200	-8.032	88.383	1.00	6.38	C
ATOM 1451	C THR G 373	33.254	-9.236	88.503	1.00	6.11	C
ATOM 1452	O THR G 373	32.762	-9.720	87.489	1.00	7.72	O
ATOM 1453	CB THR G 373	33.440	-6.717	88.796	1.00	3.53	C

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FIG. 53-29	ATOM 1455	CG2 THR G 373	34.341	-5.514	88.499	1.00	2.00	C
	ATOM 1456	N HIS G 374	33.034	-9.737	89.721	1.00	5.67	N
	ATOM 1457	CA HIS G 374	32.119	-10.868	89.931	1.00	7.82	C
	ATOM 1458	C HIS G 374	30.696	-10.362	89.714	1.00	9.15	C
	ATOM 1459	O HIS G 374	30.019	-9.989	90.667	1.00	10.34	O
	ATOM 1460	CB HIS G 374	32.259	-11.466	91.362	1.00	5.94	C
	ATOM 1461	CG HIS G 374	31.164	-12.434	91.746	1.00	6.61	C
	ATOM 1462	ND1 HIS G 374	30.810	-13.523	90.976	1.00	4.93	N
	ATOM 1463	CD2 HIS G 374	30.312	-12.444	92.803	1.00	6.52	C
	ATOM 1464	CE1 HIS G 374	29.786	-14.148	91.527	1.00	2.00	C
	ATOM 1465	NE2 HIS G 374	29.464	-13.516	92.641	1.00	2.00	N
	ATOM 1466	N SER G 375	30.256	-10.317	88.462	1.00	10.09	N
	ATOM 1467	CA SER G 375	28.906	-9.852	88.149	1.00	10.24	C
	ATOM 1468	C SER G 375	27.942	-11.016	88.248	1.00	9.46	C
	ATOM 1469	O SER G 375	28.258	-12.147	87.866	1.00	9.82	O
	ATOM 1470	CB SER G 375	28.848	-9.240	86.749	1.00	11.18	C
	ATOM 1471	OG SER G 375	29.837	-8.236	86.596	1.00	14.87	O
	ATOM 1472	N PHE G 376	26.755	-10.739	88.752	1.00	8.32	N
	ATOM 1473	CA PHE G 376	25.750	-11.767	88.920	1.00	8.62	C
	ATOM 1474	C PHE G 376	24.419	-11.086	89.133	1.00	9.88	C
	ATOM 1475	O PHE G 376	24.358	-9.868	89.298	1.00	9.95	O
	ATOM 1476	CB PHE G 376	26.085	-12.633	90.144	1.00	8.97	C
	ATOM 1477	CG PHE G 376	26.292	-11.848	91.412	1.00	6.84	C
	ATOM 1478	CD1 PHE G 376	27.530	-11.271	91.692	1.00	4.82	C
	ATOM 1479	CD2 PHE G 376	25.245	-11.662	92.314	1.00	5.82	C
	ATOM 1480	CE1 PHE G 376	27.727	-10.523	92.848	1.00	2.00	C
	ATOM 1481	CE2 PHE G 376	25.429	-10.918	93.470	1.00	3.10	C
	ATOM 1482	CZ PHE G 376	26.674	-10.346	93.737	1.00	4.76	C
	ATOM 1483	N ASN G 377	23.343	-11.857	89.097	1.00	12.53	N
	ATOM 1484	CA ASN G 377	22.038	-11.266	89.317	1.00	15.48	C
	ATOM 1485	C ASN G 377	21.530	-11.603	90.706	1.00	17.28	C
	ATOM 1486	O ASN G 377	21.080	-12.717	90.963	1.00	18.65	O
	ATOM 1487	CB ASN G 377	21.019	-11.710	88.272	1.00	13.51	C
	ATOM 1488	CG ASN G 377	19.762	-10.887	88.331	1.00	11.15	C
	ATOM 1489	OD1 ASN G 377	18.847	-11.184	89.092	1.00	11.21	O
	ATOM 1490	ND2 ASN G 377	19.739	-9.803	87.578	1.00	10.80	N
	ATOM 1491	N CYS G 378	21.621	-10.643	91.610	1.00	18.56	N
	ATOM 1492	CA CYS G 378	21.156	-10.859	92.961	1.00	19.65	C
	ATOM 1493	C CYS G 378	19.777	-10.235	93.173	1.00	18.46	C
	ATOM 1494	O CYS G 378	19.574	-9.041	92.945	1.00	18.50	O
	ATOM 1495	CB CYS G 378	22.165	-10.299	93.954	1.00	23.94	C
	ATOM 1496	SG CYS G 378	21.505	-10.141	95.635	1.00	29.07	S
	ATOM 1497	N GLY G 379	18.822	-11.062	93.580	1.00	17.14	N
	ATOM 1498	CA GLY G 379	17.473	-10.589	93.825	1.00	14.59	C
	ATOM 1499	C GLY G 379	16.886	-9.817	92.665	1.00	13.25	C
	ATOM 1500	O GLY G 379	16.120	-8.879	92.880	1.00	12.24	O
	ATOM 1501	N GLY G 380	17.228	-10.205	91.439	1.00	13.61	N
	ATOM 1502	CA GLY G 380	16.716	-9.510	90.265	1.00	14.33	C
	ATOM 1503	C GLY G 380	17.650	-8.421	89.749	1.00	15.07	C
	ATOM 1504	O GLY G 380	17.717	-8.171	88.546	1.00	16.13	O
	ATOM 1505	N GLU G 381	18.383	-7.790	90.663	1.00	14.90	N
	ATOM 1506	CA GLU G 381	19.332	-6.720	90.353	1.00	13.02	C
	ATOM 1507	C GLU G 381	20.696	-7.221	89.861	1.00	10.60	C
	ATOM 1508	O GLU G 381	21.112	-8.338	90.167	1.00	11.59	O
	ATOM 1509	CB GLU G 381	19.531	-5.847	91.594	1.00	13.97	C
	ATOM 1510	CG GLU G 381	18.237	-5.322	92.190	1.00	15.75	C
	ATOM 1511	CD GLU G 381	17.441	-4.452	91.236	1.00	16.89	C
	ATOM 1512	OE1 GLU G 381	18.034	-3.590	90.556	1.00	16.68	O
	ATOM 1513	OE2 GLU G 381	16.202	-4.613	91.183	1.00	16.68	O
	ATOM 1514	N PHE G 382	21.415	-6.374	89.133	1.00	8.55	N
	ATOM 1515	CA PHE G 382	22.722	-6.749	88.602	1.00	6.61	C
	ATOM 1516	C PHE G 382	23.859	-6.180	89.437	1.00	6.22	C
	ATOM 1517	O PHE G 382	24.055	-4.970	89.471	1.00	6.06	O
	ATOM 1518	CB PHE G 382	22.860	-6.298	87.142	1.00	5.59	C
	ATOM 1519	CG PHE G 382	22.107	-7.160	86.169	1.00	3.05	C
	ATOM 1520	CD1 PHE G 382	20.777	-6.906	85.883	1.00	2.75	C
	ATOM 1521	CD2 PHE G 382	22.723	-8.253	85.567	1.00	5.74	C
	ATOM 1522	CE1 PHE G 382	20.065	-7.734	85.011	1.00	7.02	C
	ATOM 1523	CE2 PHE G 382	22.017	-9.093	84.688	1.00	5.25	C
	ATOM 1524	CG PHE G 382	20.600	-8.826	84.411	1.00	3.76	C

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FIG. 53-30

ATOM 1526	CA PHE G 383	25.717	-6.661	90.954	1.00	6.22	C
ATOM 1527	C PHE G 383	27.057	-6.759	90.221	1.00	6.64	C
ATOM 1528	O PHE G 383	27.267	-7.662	89.415	1.00	7.52	O
ATOM 1529	CB PHE G 383	25.791	-7.544	92.199	1.00	6.69	C
ATOM 1530	CG PHE G 383	24.766	-7.220	93.251	1.00	7.52	C
ATOM 1531	CD1 PHE G 383	23.405	-7.274	92.966	1.00	7.11	C
ATOM 1532	CD2 PHE G 383	25.162	-6.886	94.541	1.00	9.04	C
ATOM 1533	CE1 PHE G 383	22.449	-7.003	93.950	1.00	5.43	C
ATOM 1534	CE2 PHE G 383	24.211	-6.612	95.529	1.00	9.60	C
ATOM 1535	CZ PHE G 383	22.849	-6.673	95.224	1.00	8.15	C
ATOM 1536	N TYR G 384	27.951	-5.814	90.498	1.00	7.28	N
ATOM 1537	CA TYR G 384	29.288	-5.792	89.921	1.00	7.20	C
ATOM 1538	C TYR G 384	30.192	-5.624	91.123	1.00	9.74	C
ATOM 1539	O TYR G 384	30.443	-4.498	91.583	1.00	7.60	O
ATOM 1540	CB TYR G 384	29.467	-4.631	88.944	1.00	5.41	C
ATOM 1541	CG TYR G 384	28.790	-4.859	87.618	1.00	6.23	C
ATOM 1542	CD1 TYR G 384	27.397	-4.865	87.519	1.00	7.75	C
ATOM 1543	CD2 TYR G 384	29.532	-5.138	86.479	1.00	3.64	C
ATOM 1544	CE1 TYR G 384	26.767	-5.151	86.324	1.00	6.63	C
ATOM 1545	CE2 TYR G 384	28.910	-5.422	85.285	1.00	5.35	C
ATOM 1546	CZ TYR G 384	27.528	-5.435	85.213	1.00	7.83	C
ATOM 1547	OH TYR G 384	26.902	-5.754	84.035	1.00	9.77	O
ATOM 1548	N CYS G 385	30.596	-6.769	91.672	1.00	11.76	N
ATOM 1549	CA CYS G 385	31.444	-6.837	92.855	1.00	13.95	C
ATOM 1550	C CYS G 385	32.920	-6.827	92.532	1.00	13.31	C
ATOM 1551	O CYS G 385	33.412	-7.713	91.838	1.00	13.77	O
ATOM 1552	CB CYS G 385	31.109	-8.095	93.665	1.00	16.62	C
ATOM 1553	SG CYS G 385	30.158	-7.819	95.196	1.00	24.71	S
ATOM 1554	N ASN G 386	33.617	-5.824	93.054	1.00	14.35	N
ATOM 1555	CA ASN G 386	35.061	-5.649	92.875	1.00	14.44	C
ATOM 1556	C ASN G 386	35.779	-6.732	93.694	1.00	14.52	C
ATOM 1557	O ASN G 386	35.705	-6.730	94.926	1.00	14.97	O
ATOM 1558	CB ASN G 386	35.425	-4.231	93.337	1.00	14.08	C
ATOM 1559	CG ASN G 386	36.921	-3.995	93.467	1.00	13.06	C
ATOM 1560	OD1 ASN G 386	37.757	-4.816	93.076	1.00	12.59	O
ATOM 1561	ND2 ASN G 386	37.244	-2.849	94.062	1.00	13.67	N
ATOM 1562	N SER G 387	36.480	-7.637	93.013	1.00	13.53	N
ATOM 1563	CA SER G 387	37.143	-8.748	93.689	1.00	12.23	C
ATOM 1564	C SER G 387	38.659	-8.732	93.818	1.00	13.58	C
ATOM 1565	O SER G 387	39.256	-9.774	94.085	1.00	14.47	O
ATOM 1566	CB SER G 387	36.721	-10.068	93.042	1.00	10.53	C
ATOM 1567	OG SER G 387	37.183	-10.157	91.706	1.00	5.98	O
ATOM 1568	N THR G 388	39.299	-7.575	93.684	1.00	14.06	N
ATOM 1569	CA THR G 388	40.758	-7.530	93.794	1.00	13.25	C
ATOM 1570	C THR G 388	41.255	-8.269	95.036	1.00	13.29	C
ATOM 1571	O THR G 388	42.319	-8.878	95.013	1.00	12.96	O
ATOM 1572	CB THR G 388	41.271	-6.078	93.850	1.00	12.91	C
ATOM 1573	OG1 THR G 388	40.886	-5.391	92.651	1.00	15.59	O
ATOM 1574	CG2 THR G 388	42.798	-6.044	93.982	1.00	10.34	C
ATOM 1575	N GLN G 389	40.456	-8.242	96.101	1.00	14.26	N
ATOM 1576	CA GLN G 389	40.806	-8.876	97.377	1.00	15.10	C
ATOM 1577	C GLN G 389	40.728	-10.388	97.433	1.00	15.75	C
ATOM 1578	O GLN G 389	41.126	-10.991	98.429	1.00	16.29	O
ATOM 1579	CB GLN G 389	39.942	-8.331	98.498	1.00	14.13	C
ATOM 1580	CG GLN G 389	40.175	-6.895	98.826	1.00	11.93	C
ATOM 1581	CD GLN G 389	39.164	-6.419	99.816	1.00	13.44	C
ATOM 1582	OE1 GLN G 389	38.019	-6.150	99.456	1.00	13.89	O
ATOM 1583	NE2 GLN G 389	39.547	-6.378	101.087	1.00	12.50	N
ATOM 1584	N LEU G 390	40.135	-10.997	96.418	1.00	15.10	N
ATOM 1585	CA LEU G 390	40.032	-12.436	96.396	1.00	14.73	C
ATOM 1586	C LEU G 390	41.191	-12.988	95.581	1.00	15.84	C
ATOM 1587	O LEU G 390	41.787	-14.007	95.941	1.00	15.56	O
ATOM 1588	CB LEU G 390	38.686	-12.866	95.812	1.00	15.03	C
ATOM 1589	CG LEU G 390	37.446	-12.472	96.628	1.00	14.64	C
ATOM 1590	CD1 LEU G 390	36.183	-12.891	95.913	1.00	13.49	C
ATOM 1591	CD2 LEU G 390	37.502	-13.114	97.994	1.00	14.61	C
ATOM 1592	N PHE G 391	41.604	-12.235	94.572	1.00	16.01	N
ATOM 1593	CA PHE G 391	42.681	-12.675	93.700	1.00	17.41	C
ATOM 1594	C PHE G 391	43.886	-11.730	93.729	1.00	21.15	C
ATOM 1595	O PHE G 391	44.178	-11.066	97.795	1.00	20.08	O

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FIG. 53-31	ATOM 1597	CG PHE G 391	40.811 -13.590 92.251 1.00 12.10	C
	ATOM 1598	CD1 PHE G 391	40.781 -14.983 92.260 1.00 11.26	C
	ATOM 1599	CD2 PHE G 391	39.602 -12.895 92.225 1.00 8.89	C
	ATOM 1600	CE1 PHE G 391	39.560 -15.671 92.248 1.00 11.86	C
	ATOM 1601	CE2 PHE G 391	38.383 -13.565 92.215 1.00 6.77	C
	ATOM 1602	CZ PHE G 391	38.359 -14.955 92.223 1.00 9.67	C
	ATOM 1603	N ASN G 392	44.632 -11.783 94.826 1.00 24.97	N
	ATOM 1604	CA ASN G 392	45.813 -10.949 95.012 1.00 28.18	C
	ATOM 1605	C ASN G 392	46.600 -11.565 96.169 1.00 28.19	C
	ATOM 1606	O ASN G 392	46.477 -11.153 97.325 1.00 29.12	O
	ATOM 1607	CB ASN G 392	45.395 -9.506 95.323 1.00 32.77	C
	ATOM 1608	CG ASN G 392	46.577 -8.546 95.383 1.00 38.54	C
	ATOM 1609	OD1 ASN G 392	47.067 -8.096 94.343 1.00 38.50	O
	ATOM 1610	ND2 ASN G 392	47.055 -8.234 96.588 1.00 43.33	N
	ATOM 1611	N SER G 393	47.396 -12.577 95.851 1.00 26.88	N
	ATOM 1612	CA SER G 393	48.180 -13.271 96.857 1.00 25.07	C
	ATOM 1613	C SER G 393	49.251 -14.104 96.188 1.00 24.68	C
	ATOM 1614	O SER G 393	49.289 -14.200 94.963 1.00 24.20	O
	ATOM 1615	CB SER G 393	47.267 -14.178 97.668 1.00 24.54	C
	ATOM 1616	OG SER G 393	46.466 -14.977 96.815 1.00 24.25	O
	ATOM 1617	N THR G 394	50.128 -14.695 96.991 1.00 24.89	N
	ATOM 1618	CA THR G 394	51.188 -15.531 96.457 1.00 25.72	C
	ATOM 1619	C THR G 394	51.357 -16.790 97.299 1.00 26.39	C
	ATOM 1620	O THR G 394	51.173 -16.770 98.522 1.00 25.65	O
	ATOM 1621	CB THR G 394	52.512 -14.781 96.365 1.00 24.64	C
	ATOM 1622	OG1 THR G 394	52.287 -13.492 95.782 1.00 24.17	O
	ATOM 1623	CG2 THR G 394	53.471 -15.548 95.485 1.00 24.29	C
	ATOM 1624	N TRP G 395	51.654 -17.890 96.613 1.00 26.26	N
	ATOM 1625	CA TRP G 395	51.832 -19.191 97.235 1.00 25.14	C
	ATOM 1626	C TRP G 395	52.914 -19.942 96.475 1.00 26.41	C
	ATOM 1627	O TRP G 395	53.501 -19.434 95.510 1.00 26.05	O
	ATOM 1628	CB TRP G 395	50.543 -20.022 97.138 1.00 22.22	C
	ATOM 1629	CG TRP G 395	49.262 -19.274 97.377 1.00 19.31	C
	ATOM 1630	CD1 TRP G 395	48.617 -18.447 96.497 1.00 16.61	C
	ATOM 1631	CD2 TRP G 395	48.454 -19.308 98.562 1.00 16.61	C
	ATOM 1632	NE1 TRP G 395	47.463 -17.969 97.062 1.00 16.86	N
	ATOM 1633	CE2 TRP G 395	47.336 -18.479 98.328 1.00 14.88	C
	ATOM 1634	CE3 TRP G 395	48.566 -19.956 99.798 1.00 16.95	C
	ATOM 1635	CZ2 TRP G 395	46.334 -18.286 99.280 1.00 12.10	C
	ATOM 1636	CZ3 TRP G 395	47.560 -19.761 100.752 1.00 15.27	C
	ATOM 1637	CH2 TRP G 395	46.463 -18.931 100.482 1.00 14.32	C
	ATOM 1638	N PHE G 396	53.155 -21.174 96.902 1.00 27.88	N
	ATOM 1639	CA PHE G 396	54.145 -22.031 96.262 1.00 28.86	C
	ATOM 1640	C PHE G 396	53.534 -23.428 96.176 1.00 27.43	C
	ATOM 1641	O PHE G 396	52.313 -23.576 96.300 1.00 26.00	O
	ATOM 1642	CB PHE G 396	55.458 -22.043 97.066 1.00 30.01	C
	ATOM 1643	CG PHE G 396	56.096 -20.681 97.217 1.00 29.71	C
	ATOM 1644	CD1 PHE G 396	56.966 -20.200 96.256 1.00 30.49	C
	ATOM 1645	CD2 PHE G 396	55.815 -19.880 98.316 1.00 31.10	C
	ATOM 1646	CE1 PHE G 396	57.549 -18.939 96.379 1.00 31.47	C
	ATOM 1647	CE2 PHE G 396	56.396 -18.613 98.447 1.00 32.07	C
	ATOM 1648	CZ PHE G 396	57.262 -18.146 97.475 1.00 30.57	C
	ATOM 1649	N GLY G 410	39.849 -12.755 114.824 1.00 52.61	N
	ATOM 1650	CA GLY G 410	38.587 -13.108 115.447 1.00 52.39	C
	ATOM 1651	C GLY G 410	37.505 -13.439 114.438 1.00 52.68	C
	ATOM 1652	O GLY G 410	37.211 -14.611 114.187 1.00 52.57	O
	ATOM 1653	N SER G 411	36.904 -12.405 113.859 1.00 52.15	N
	ATOM 1654	CA SER G 411	35.853 -12.596 112.868 1.00 50.82	C
	ATOM 1655	C SER G 411	36.158 -11.719 111.649 1.00 49.37	C
	ATOM 1656	O SER G 411	35.352 -10.878 111.241 1.00 49.20	O
	ATOM 1657	CB SER G 411	34.488 -12.252 113.479 1.00 50.78	C
	ATOM 1658	OG SER G 411	33.416 -12.697 112.661 1.00 52.19	O
	ATOM 1659	N ASP G 412	37.344 -11.920 111.087 1.00 47.75	N
	ATOM 1660	CA ASP G 412	37.805 -11.170 109.923 1.00 46.28	C
	ATOM 1661	C ASP G 412	37.092 -11.612 108.649 1.00 44.08	C
	ATOM 1662	O ASP G 412	37.242 -12.761 108.214 1.00 44.81	O
	ATOM 1663	CB ASP G 412	39.312 -11.373 109.738 1.00 49.02	C
	ATOM 1664	CG ASP G 412	40.144 -10.671 110.801 1.00 51.99	C
	ATOM 1665	OD1 ASP G 412	40.479 -9.476 110.608 1.00 53.47	O
	ATOM 1666	ND2 ASP G 412	40.486 -11.324 111.811 1.00 54.16	O



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FIG. 53-32	ATOM 1668	CA THR G 413	35.584	-11.026	106.828	1.00	35.17	C
	ATOM 1669	C THR G 413	36.110	-10.208	105.646	1.00	32.12	C
	ATOM 1670	O THR G 413	36.544	-9.060	105.808	1.00	31.22	O
	ATOM 1671	CB THR G 413	34.054	-10.813	106.972	1.00	33.87	C
	ATOM 1672	OG1 THR G 413	33.792	-9.594	107.672	1.00	32.02	O
	ATOM 1673	CG2 THR G 413	33.429	-11.959	107.732	1.00	34.44	C
	ATOM 1674	N ILE G 414	36.159	-10.843	104.479	1.00	28.34	N
	ATOM 1675	CA ILE G 414	36.614	-10.187	103.268	1.00	24.52	C
	ATOM 1676	C ILE G 414	35.458	-9.380	102.705	1.00	22.34	C
	ATOM 1677	O ILE G 414	34.510	-9.945	102.153	1.00	20.15	O
	ATOM 1678	CB ILE G 414	37.067	-11.193	102.190	1.00	24.43	C
	ATOM 1679	CG1 ILE G 414	38.277	-11.992	102.671	1.00	23.83	C
	ATOM 1680	CG2 ILE G 414	37.413	-10.455	100.908	1.00	23.71	C
	ATOM 1681	CD1 ILE G 414	38.858	-12.924	101.622	1.00	23.64	C
	ATOM 1682	N THR G 415	35.510	-8.066	102.921	1.00	21.24	N
	ATOM 1683	CA THR G 415	34.487	-7.161	102.417	1.00	19.23	C
	ATOM 1684	C THR G 415	34.843	-6.756	100.989	1.00	18.99	C
	ATOM 1685	O THR G 415	35.941	-6.267	100.726	1.00	19.68	O
	ATOM 1686	CB THR G 415	34.359	-5.913	103.301	1.00	17.55	C
	ATOM 1687	OG1 THR G 415	33.746	-6.276	104.542	1.00	18.24	O
	ATOM 1688	CG2 THR G 415	33.519	-4.857	102.627	1.00	16.11	C
	ATOM 1689	N LEU G 416	33.923	-7.010	100.070	1.00	16.60	N
	ATOM 1690	CA LEU G 416	34.114	-6.680	98.665	1.00	14.46	C
	ATOM 1691	C LEU G 416	33.161	-5.564	98.278	1.00	12.35	C
	ATOM 1692	O LEU G 416	31.959	-5.635	98.573	1.00	9.32	O
	ATOM 1693	CB LEU G 416	33.799	-7.902	97.797	1.00	15.19	C
	ATOM 1694	CG LEU G 416	34.873	-8.761	97.133	1.00	14.82	C
	ATOM 1695	CD1 LEU G 416	36.074	-8.962	98.035	1.00	17.46	C
	ATOM 1696	CD2 LEU G 416	34.250	-10.088	96.759	1.00	13.29	C
	ATOM 1697	N PRO G 417	33.694	-4.480	97.686	1.00	11.52	N
	ATOM 1698	CA PRO G 417	32.875	-3.348	97.251	1.00	11.96	C
	ATOM 1699	C PRO G 417	32.049	-3.903	96.094	1.00	12.68	C
	ATOM 1700	O PRO G 417	32.588	-4.602	95.228	1.00	12.98	O
	ATOM 1701	CB PRO G 417	33.914	-2.352	96.724	1.00	12.10	C
	ATOM 1702	CG PRO G 417	35.173	-2.740	97.406	1.00	11.06	C
	ATOM 1703	CD PRO G 417	35.117	-4.228	97.412	1.00	11.57	C
	ATOM 1704	N CYS G 418	30.785	-3.525	96.025	1.00	13.47	N
	ATOM 1705	CA CYS G 418	29.897	-4.023	94.992	1.00	15.31	C
	ATOM 1706	C CYS G 418	29.086	-2.853	94.435	1.00	16.22	C
	ATOM 1707	O CYS G 418	28.928	-1.832	95.101	1.00	17.53	O
	ATOM 1708	CB CYS G 418	28.964	-5.049	95.618	1.00	16.68	C
	ATOM 1709	SG CYS G 418	28.665	-6.556	94.655	1.00	21.94	S
	ATOM 1710	N ARG G 419	28.585	-2.992	93.211	1.00	16.78	N
	ATOM 1711	CA ARG G 419	27.794	-1.932	92.582	1.00	16.62	C
	ATOM 1712	C ARG G 419	26.685	-2.521	91.720	1.00	16.08	C
	ATOM 1713	O ARG G 419	26.903	-3.504	91.021	1.00	16.64	O
	ATOM 1714	CB ARG G 419	28.678	-1.007	91.717	1.00	15.68	C
	ATOM 1715	CG ARG G 419	27.936	0.239	91.257	1.00	20.03	C
	ATOM 1716	CD ARG G 419	28.752	1.214	90.415	1.00	24.39	C
	ATOM 1717	NE ARG G 419	27.968	2.426	90.131	1.00	29.10	N
	ATOM 1718	CZ ARG G 419	28.476	3.651	89.974	1.00	30.37	C
	ATOM 1719	NH1 ARG G 419	29.785	3.855	90.060	1.00	29.71	N
	ATOM 1720	NH2 ARG G 419	27.664	4.697	89.829	1.00	29.99	N
	ATOM 1721	N ILE G 420	25.502	-1.919	91.782	1.00	15.40	N
	ATOM 1722	CA ILE G 420	24.355	-2.359	91.001	1.00	13.99	C
	ATOM 1723	C ILE G 420	24.247	-1.458	89.773	1.00	15.21	C
	ATOM 1724	O ILE G 420	23.988	-0.256	89.900	1.00	17.67	O
	ATOM 1725	CB ILE G 420	23.070	-2.217	91.808	1.00	13.88	C
	ATOM 1726	CG1 ILE G 420	23.269	-2.795	93.211	1.00	15.98	C
	ATOM 1727	CG2 ILE G 420	21.924	-2.926	91.115	1.00	11.82	C
	ATOM 1728	CD1 ILE G 420	22.137	-2.455	94.195	1.00	19.11	C
	ATOM 1729	N LYS G 421	24.487	-2.021	88.593	1.00	13.87	N
	ATOM 1730	CA LYS G 421	24.405	-1.255	87.356	1.00	11.70	C
	ATOM 1731	C LYS G 421	23.091	-1.534	86.641	1.00	13.43	C
	ATOM 1732	O LYS G 421	22.480	-2.591	86.828	1.00	14.32	O
	ATOM 1733	CB LYS G 421	25.583	-1.585	86.443	1.00	8.86	C
	ATOM 1734	CG LYS G 421	26.930	-1.279	87.064	1.00	5.47	C
	ATOM 1735	CD LYS G 421	28.061	-1.414	86.066	1.00	2.59	C
	ATOM 1736	CE LYS G 421	29.387	-1.115	86.741	1.00	2.00	C
	ATOM 1737	N LYS G 421	20.474	0.900	85.774	1.00	2.10	N

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FIG. 53-33	ATOM 1739 CA GLN G 422	21.397	-0.709	85.101	1.00	13.90	C
	ATOM 1740 C GLN G 422	21.673	-0.955	83.610	1.00	14.50	C
	ATOM 1741 O GLN G 422	20.943	-1.713	82.958	1.00	15.64	O
	ATOM 1742 CB GLN G 422	20.494	0.506	85.322	1.00	12.83	C
	ATOM 1743 CG GLN G 422	19.847	0.535	86.717	1.00	14.26	C
	ATOM 1744 CD GLN G 422	20.518	1.500	87.700	1.00	14.75	C
	ATOM 1745 OE1 GLN G 422	20.787	2.652	87.368	1.00	16.42	O
	ATOM 1746 NE2 GLN G 422	20.765	1.035	88.921	1.00	13.83	N
	ATOM 1747 N ILE G 423	22.732	-0.339	83.085	1.00	13.65	N
	ATOM 1748 CA ILE G 423	23.129	-0.515	81.686	1.00	12.75	C
	ATOM 1749 C ILE G 423	24.195	-1.611	81.697	1.00	12.32	C
	ATOM 1750 O ILE G 423	25.281	-1.415	82.239	1.00	12.02	O
	ATOM 1751 CB ILE G 423	23.814	0.744	81.086	1.00	12.86	C
	ATOM 1752 CG1 ILE G 423	23.001	2.025	81.344	1.00	13.94	C
	ATOM 1753 CG2 ILE G 423	24.057	0.529	79.614	1.00	12.18	C
	ATOM 1754 CD1 ILE G 423	21.708	2.151	80.554	1.00	14.57	C
	ATOM 1755 N ILE G 424	23.912	-2.743	81.063	1.00	11.96	N
	ATOM 1756 CA ILE G 424	24.867	-3.850	81.036	1.00	10.17	C
	ATOM 1757 C ILE G 424	25.153	-4.381	79.639	1.00	9.57	C
	ATOM 1758 O ILE G 424	24.355	-4.202	78.719	1.00	10.04	O
	ATOM 1759 CB ILE G 424	24.346	-5.031	81.881	1.00	6.45	C
	ATOM 1760 CG1 ILE G 424	22.906	-5.363	81.463	1.00	6.31	C
	ATOM 1761 CG2 ILE G 424	24.379	-4.671	83.343	1.00	4.81	C
	ATOM 1762 CD1 ILE G 424	22.384	-6.680	81.976	1.00	5.79	C
	ATOM 1763 N ASN G 425	26.325	-4.980	79.471	1.00	10.25	N
	ATOM 1764 CA ASN G 425	26.692	-5.611	78.204	1.00	10.60	C
	ATOM 1765 C ASN G 425	26.048	-6.998	78.349	1.00	10.47	C
	ATOM 1766 O ASN G 425	26.174	-7.641	79.400	1.00	10.16	O
	ATOM 1767 CB ASN G 425	28.212	-5.763	78.090	1.00	12.33	C
	ATOM 1768 CG ASN G 425	28.939	-4.427	78.007	1.00	15.15	C
	ATOM 1769 OD1 ASN G 425	28.652	-3.607	77.130	1.00	17.02	O
	ATOM 1770 ND2 ASN G 425	29.903	-4.213	78.898	1.00	12.02	N
	ATOM 1771 N MET G 426	25.319	-7.444	77.335	1.00	11.26	N
	ATOM 1772 CA MET G 426	24.661	-8.752	77.411	1.00	11.94	C
	ATOM 1773 C MET G 426	25.623	-9.929	77.323	1.00	11.81	C
	ATOM 1774 O MET G 426	26.686	-9.839	76.694	1.00	10.19	O
	ATOM 1775 CB MET G 426	23.612	-8.910	76.305	1.00	11.27	C
	ATOM 1776 CG MET G 426	22.518	-7.882	76.300	1.00	11.33	C
	ATOM 1777 SD MET G 426	21.617	-7.901	74.730	1.00	12.85	S
	ATOM 1778 CE MET G 426	20.042	-8.430	75.332	1.00	13.82	C
	ATOM 1779 N TRP G 427	25.226	-11.030	77.961	1.00	12.45	N
	ATOM 1780 CA TRP G 427	25.995	-12.273	77.938	1.00	11.41	C
	ATOM 1781 C TRP G 427	25.385	-13.206	76.878	1.00	11.82	C
	ATOM 1782 O TRP G 427	26.056	-14.083	76.348	1.00	11.82	O
	ATOM 1783 CB TRP G 427	25.977	-12.954	79.319	1.00	10.11	C
	ATOM 1784 CG TRP G 427	24.631	-13.502	79.756	1.00	7.53	C
	ATOM 1785 CD1 TRP G 427	23.711	-12.877	80.542	1.00	8.23	C
	ATOM 1786 CD2 TRP G 427	24.046	-14.769	79.392	1.00	7.92	C
	ATOM 1787 NE1 TRP G 427	22.589	-13.658	80.684	1.00	8.61	N
	ATOM 1788 CE2 TRP G 427	22.765	-14.824	79.988	1.00	7.83	C
	ATOM 1789 CE3 TRP G 427	24.477	-15.860	78.617	1.00	4.40	C
	ATOM 1790 CZ2 TRP G 427	21.907	-15.927	79.834	1.00	4.16	C
	ATOM 1791 CZ3 TRP G 427	23.626	-16.953	78.466	1.00	3.07	C
	ATOM 1792 CH2 TRP G 427	22.354	-16.974	79.074	1.00	3.36	C
	ATOM 1793 N GLN G 428	24.102	-13.002	76.578	1.00	12.92	N
	ATOM 1794 CA GLN G 428	23.383	-13.819	75.602	1.00	12.50	C
	ATOM 1795 C GLN G 428	23.995	-13.688	74.226	1.00	12.17	C
	ATOM 1796 O GLN G 428	24.340	-14.686	73.592	1.00	12.46	O
	ATOM 1797 CB GLN G 428	21.907	-13.410	75.532	1.00	13.40	C
	ATOM 1798 CG GLN G 428	21.076	-13.744	76.776	1.00	17.89	C
	ATOM 1799 CD GLN G 428	20.660	-12.520	77.570	1.00	17.31	C
	ATOM 1800 OE1 GLN G 428	21.457	-11.608	77.793	1.00	19.51	O
	ATOM 1801 NE2 GLN G 428	19.418	-12.501	78.012	1.00	16.89	N
	ATOM 1802 N LYS G 429	24.126	-12.440	73.781	1.00	12.47	N
	ATOM 1803 CA LYS G 429	24.676	-12.096	72.472	1.00	11.30	C
	ATOM 1804 C LYS G 429	25.355	-10.737	72.649	1.00	11.73	C
	ATOM 1805 O LYS G 429	25.245	-10.134	73.720	1.00	11.55	O
	ATOM 1806 CB LYS G 429	23.541	-12.013	71.443	1.00	10.96	C
	ATOM 1807 CG LYS G 429	22.583	-10.847	71.655	1.00	10.29	C
	ATOM 1808 CD LYS G 429	21.734	-11.049	70.963	1.00	9.65	C

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FIG. 53-34	ATOM 1810 NZ LYS G 429	18.772	-11.467	71.526	1.00	14.65	N
	ATOM 1811 N VAL G 430	26.075	-10.266	71.630	1.00	12.29	N
	ATOM 1812 CA VAL G 430	26.763	-8.976	71.727	1.00	11.03	C
	ATOM 1813 C VAL G 430	25.778	-7.819	71.695	1.00	12.15	C
	ATOM 1814 O VAL G 430	25.471	-7.269	70.635	1.00	13.94	O
	ATOM 1815 CB VAL G 430	27.835	-8.792	70.629	1.00	9.34	C
	ATOM 1816 CG1 VAL G 430	28.306	-7.345	70.578	1.00	7.26	C
	ATOM 1817 CG2 VAL G 430	29.025	-9.687	70.908	1.00	7.39	C
	ATOM 1818 N GLY G 431	25.288	-7.450	72.869	1.00	11.73	N
	ATOM 1819 CA GLY G 431	24.335	-6.364	72.956	1.00	11.01	C
	ATOM 1820 C GLY G 431	24.505	-5.575	74.235	1.00	10.82	C
	ATOM 1821 O GLY G 431	25.433	-5.820	75.027	1.00	9.94	O
	ATOM 1822 N LYS G 432	23.594	-4.630	74.432	1.00	9.68	N
	ATOM 1823 CA LYS G 432	23.583	-3.761	75.597	1.00	10.19	C
	ATOM 1824 C LYS G 432	22.130	-3.740	76.066	1.00	10.15	C
	ATOM 1825 O LYS G 432	21.218	-3.913	75.251	1.00	11.95	O
	ATOM 1826 CB LYS G 432	24.021	-2.355	75.168	1.00	12.15	C
	ATOM 1827 CG LYS G 432	24.193	-1.330	76.284	1.00	12.45	C
	ATOM 1828 CD LYS G 432	25.407	-1.624	77.142	1.00	13.71	C
	ATOM 1829 CE LYS G 432	26.671	-1.729	76.308	1.00	14.39	C
	ATOM 1830 NZ LYS G 432	26.857	-0.585	75.395	1.00	16.43	N
	ATOM 1831 N ALA G 433	21.904	-3.576	77.364	1.00	8.77	N
	ATOM 1832 CA ALA G 433	20.544	-3.536	77.889	1.00	7.95	C
	ATOM 1833 C ALA G 433	20.465	-2.606	79.095	1.00	8.53	C
	ATOM 1834 O ALA G 433	21.481	-2.329	79.734	1.00	9.95	O
	ATOM 1835 CB ALA G 433	20.076	-4.933	78.253	1.00	5.09	C
	ATOM 1836 N MET G 434	19.273	-2.082	79.367	1.00	8.52	N
	ATOM 1837 CA MET G 434	19.063	-1.176	80.492	1.00	8.68	C
	ATOM 1838 C MET G 434	17.835	-1.608	81.263	1.00	8.39	C
	ATOM 1839 O MET G 434	16.775	-1.822	80.674	1.00	10.62	O
	ATOM 1840 CB MET G 434	18.860	0.260	79.993	1.00	12.16	C
	ATOM 1841 CG MET G 434	18.402	1.263	81.072	1.00	13.05	C
	ATOM 1842 SD MET G 434	18.040	2.931	80.444	1.00	14.02	S
	ATOM 1843 CE MET G 434	16.368	2.691	79.882	1.00	7.69	C
	ATOM 1844 N TYR G 435	17.980	-1.758	82.570	1.00	6.27	N
	ATOM 1845 CA TYR G 435	16.868	-2.156	83.409	1.00	7.78	C
	ATOM 1846 C TYR G 435	16.482	-1.020	84.369	1.00	9.51	C
	ATOM 1847 O TYR G 435	17.229	-0.060	84.556	1.00	8.60	O
	ATOM 1848 CB TYR G 435	17.221	-3.423	84.192	1.00	8.02	C
	ATOM 1849 CG TYR G 435	17.475	-4.648	83.334	1.00	6.79	C
	ATOM 1850 CD1 TYR G 435	18.682	-4.811	82.646	1.00	7.18	C
	ATOM 1851 CD2 TYR G 435	16.513	-5.648	83.218	1.00	6.66	C
	ATOM 1852 CE1 TYR G 435	18.922	-5.939	81.862	1.00	3.85	C
	ATOM 1853 CE2 TYR G 435	16.745	-6.785	82.435	1.00	6.36	C
	ATOM 1854 CZ TYR G 435	17.950	-6.919	81.761	1.00	4.00	C
	ATOM 1855 OH TYR G 435	18.160	-8.019	80.975	1.00	2.00	O
	ATOM 1856 N ALA G 436	15.299	-1.119	84.958	1.00	10.38	N
	ATOM 1857 CA ALA G 436	14.840	-0.104	85.891	1.00	11.10	C
	ATOM 1858 C ALA G 436	15.688	-0.137	87.162	1.00	11.27	C
	ATOM 1859 O ALA G 436	16.372	-1.126	87.435	1.00	11.03	O
	ATOM 1860 CB ALA G 436	13.388	-0.347	86.234	1.00	9.64	C
	ATOM 1861 N PRO G 437	15.711	0.972	87.914	1.00	11.91	N
	ATOM 1862 CA PRO G 437	16.489	1.027	89.160	1.00	11.96	C
	ATOM 1863 C PRO G 437	15.778	0.190	90.231	1.00	14.06	C
	ATOM 1864 O PRO G 437	14.629	-0.223	90.041	1.00	14.86	O
	ATOM 1865 CB PRO G 437	16.466	2.519	89.509	1.00	10.51	C
	ATOM 1866 CG PRO G 437	16.373	3.175	88.165	1.00	11.89	C
	ATOM 1867 CD PRO G 437	15.327	2.328	87.482	1.00	11.18	C
	ATOM 1868 N PRO G 438	16.447	-0.084	91.364	1.00	15.61	N
	ATOM 1869 CA PRO G 438	15.808	-0.878	92.409	1.00	16.39	C
	ATOM 1870 C PRO G 438	14.573	-0.220	93.012	1.00	17.69	C
	ATOM 1871 O PRO G 438	14.380	0.990	92.898	1.00	19.30	O
	ATOM 1872 CB PRO G 438	16.908	-0.988	93.466	1.00	15.98	C
	ATOM 1873 CG PRO G 438	18.166	-0.894	92.676	1.00	15.96	C
	ATOM 1874 CD PRO G 438	17.846	0.215	91.724	1.00	15.89	C
	ATOM 1875 N ILE G 439	13.729	-1.042	93.628	1.00	17.73	N
	ATOM 1876 CA ILE G 439	12.528	-0.583	94.320	1.00	18.43	C
	ATOM 1877 C ILE G 439	12.611	-1.061	95.772	1.00	20.45	C
	ATOM 1878 O ILE G 439	12.038	-0.457	96.675	1.00	21.24	O
	ATOM 1879 CB ILE G 439	11.246	-1.135	93.607	1.00	17.20	C

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FIG. 53-35

ATOM 1881	CG2 ILE G 439	10.967	-0.438	92.389	1.00	18.43	C
ATOM 1882	CD1 ILE G 439	10.104	-3.259	92.950	1.00	18.43	C
ATOM 1883	N SER G 440	13.349	-2.148	95.984	1.00	21.82	N
ATOM 1884	CA SER G 440	13.536	-2.723	97.306	1.00	21.89	C
ATOM 1885	C SER G 440	14.721	-2.063	97.992	1.00	22.21	C
ATOM 1886	O SER G 440	15.688	-1.671	97.334	1.00	21.84	O
ATOM 1887	CB SER G 440	13.787	-4.224	97.182	1.00	22.41	C
ATOM 1888	OG SER G 440	14.322	-4.774	98.376	1.00	24.55	O
ATOM 1889	N GLY G 441	14.645	-1.963	99.316	1.00	22.89	N
ATOM 1890	CA GLY G 441	15.717	-1.364	100.087	1.00	24.15	C
ATOM 1891	C GLY G 441	16.437	-2.406	100.918	1.00	25.78	C
ATOM 1892	O GLY G 441	17.183	-2.083	101.850	1.00	25.75	O
ATOM 1893	N GLN G 442	16.223	-3.669	100.565	1.00	27.91	N
ATOM 1894	CA GLN G 442	16.835	-4.791	101.271	1.00	27.60	C
ATOM 1895	C GLN G 442	17.094	-5.945	100.305	1.00	26.17	C
ATOM 1896	O GLN G 442	16.502	-7.011	100.433	1.00	25.20	O
ATOM 1897	CB GLN G 442	15.919	-5.256	102.413	1.00	27.55	C
ATOM 1898	CG GLN G 442	16.520	-5.156	103.818	1.00	30.75	C
ATOM 1899	CD GLN G 442	17.699	-6.102	104.055	1.00	32.94	C
ATOM 1900	OE1 GLN G 442	18.557	-5.851	104.913	1.00	33.70	O
ATOM 1901	NE2 GLN G 442	17.744	-7.191	103.302	1.00	32.33	N
ATOM 1902	N ILE G 443	17.917	-5.691	99.291	1.00	25.88	N
ATOM 1903	CA ILE G 443	18.284	-6.717	98.309	1.00	25.15	C
ATOM 1904	C ILE G 443	19.295	-7.570	99.094	1.00	25.50	C
ATOM 1905	O ILE G 443	20.334	-7.059	99.526	1.00	25.38	O
ATOM 1906	CB ILE G 443	18.978	-6.092	97.062	1.00	24.00	C
ATOM 1907	CG1 ILE G 443	18.131	-4.955	96.465	1.00	22.92	C
ATOM 1908	CG2 ILE G 443	19.268	-7.158	96.029	1.00	24.67	C
ATOM 1909	CD1 ILE G 443	16.814	-5.382	95.843	1.00	18.91	C
ATOM 1910	N ARG G 444	18.988	-8.845	99.295	1.00	25.73	N
ATOM 1911	CA ARG G 444	19.844	-9.719	100.090	1.00	24.77	C
ATOM 1912	C ARG G 444	20.013	-11.113	99.508	1.00	23.92	C
ATOM 1913	O ARG G 444	19.042	-11.862	99.390	1.00	23.58	O
ATOM 1914	CB ARG G 444	19.250	-9.830	101.498	1.00	26.54	C
ATOM 1915	CG ARG G 444	17.726	-9.982	101.485	1.00	30.41	C
ATOM 1916	CD ARG G 444	17.125	-10.040	102.877	1.00	33.05	C
ATOM 1917	NE ARG G 444	17.435	-11.298	103.545	1.00	37.05	N
ATOM 1918	CZ ARG G 444	17.082	-11.597	104.789	1.00	37.64	C
ATOM 1919	NH1 ARG G 444	16.403	-10.723	105.522	1.00	39.42	N
ATOM 1920	NH2 ARG G 444	17.411	-12.776	105.291	1.00	37.67	N
ATOM 1921	N CYS G 445	21.251	-11.474	99.185	1.00	23.87	N
ATOM 1922	CA CYS G 445	21.550	-12.791	98.634	1.00	23.58	C
ATOM 1923	C CYS G 445	22.575	-13.530	99.472	1.00	22.82	C
ATOM 1924	O CYS G 445	23.410	-12.918	100.147	1.00	23.70	O
ATOM 1925	CB CYS G 445	22.060	-12.682	97.195	1.00	25.38	C
ATOM 1926	SG CYS G 445	20.832	-12.019	96.022	1.00	31.32	S
ATOM 1927	N SER G 446	22.485	-14.853	99.456	1.00	21.52	N
ATOM 1928	CA SER G 446	23.421	-15.696	100.185	1.00	19.95	C
ATOM 1929	C SER G 446	23.700	-16.850	99.253	1.00	17.57	C
ATOM 1930	O SER G 446	22.868	-17.742	99.097	1.00	18.36	O
ATOM 1931	CB SER G 446	22.794	-16.200	101.485	1.00	22.42	C
ATOM 1932	OG SER G 446	22.326	-15.120	102.285	1.00	28.19	O
ATOM 1933	N SER G 447	24.832	-16.787	98.566	1.00	15.58	N
ATOM 1934	CA SER G 447	25.202	-17.837	97.632	1.00	13.44	C
ATOM 1935	C SER G 447	26.382	-18.658	98.123	1.00	12.68	C
ATOM 1936	O SER G 447	27.125	-18.248	99.004	1.00	10.83	O
ATOM 1937	CB SER G 447	25.499	-17.260	96.241	1.00	11.95	C
ATOM 1938	OG SER G 447	24.318	-17.164	95.462	1.00	5.00	O
ATOM 1939	N ASN G 448	26.502	-19.857	97.583	1.00	14.33	N
ATOM 1940	CA ASN G 448	27.592	-20.732	97.944	1.00	16.20	C
ATOM 1941	C ASN G 448	28.564	-20.854	96.769	1.00	14.81	C
ATOM 1942	O ASN G 448	28.198	-21.316	95.682	1.00	12.34	O
ATOM 1943	CB ASN G 448	27.063	-22.108	98.375	1.00	20.92	C
ATOM 1944	CG ASN G 448	26.868	-22.214	99.891	1.00	27.83	C
ATOM 1945	OD1 ASN G 448	27.851	-22.275	100.635	1.00	26.42	O
ATOM 1946	ND2 ASN G 448	25.612	-22.222	100.347	1.00	33.87	N
ATOM 1947	N ILE G 449	29.767	-20.316	96.948	1.00	12.69	N
ATOM 1948	CA ILE G 449	30.771	-20.423	95.916	1.00	10.25	C
ATOM 1949	C ILE G 449	31.025	-21.918	95.872	1.00	10.75	C
ATOM 1950	O ILE G 449	31.228	-22.565	96.897	1.00	9.42	O

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FIG. 53-36

ATOM 1952	CG1 ILE G 449	31.801	-18.194	96.450	1.00	8.41	C
ATOM 1953	CG2 ILE G 449	33.103	-19.885	95.166	1.00	6.30	C
ATOM 1954	CD1 ILE G 449	33.069	-17.378	96.702	1.00	8.72	C
ATOM 1955	N THR G 450	30.879	-22.460	94.680	1.00	12.00	N
ATOM 1956	CA THR G 450	31.054	-23.871	94.419	1.00	11.69	C
ATOM 1957	C THR G 450	32.246	-24.034	93.475	1.00	11.98	C
ATOM 1958	O THR G 450	32.760	-25.135	93.291	1.00	13.25	O
ATOM 1959	CB THR G 450	29.765	-24.414	93.770	1.00	13.06	C
ATOM 1960	OG1 THR G 450	28.777	-24.683	94.788	1.00	12.93	O
ATOM 1961	CG2 THR G 450	30.047	-25.633	92.922	1.00	13.57	C
ATOM 1962	N GLY G 451	32.712	-22.928	92.906	1.00	11.41	N
ATOM 1963	CA GLY G 451	33.839	-23.018	92.004	1.00	10.26	C
ATOM 1964	C GLY G 451	34.587	-21.735	91.708	1.00	8.61	C
ATOM 1965	O GLY G 451	34.510	-20.749	92.440	1.00	8.05	O
ATOM 1966	N LEU G 452	35.291	-21.757	90.587	1.00	7.27	N
ATOM 1967	CA LEU G 452	36.095	-20.640	90.148	1.00	7.77	C
ATOM 1968	C LEU G 452	36.388	-20.911	88.677	1.00	6.70	C
ATOM 1969	O LEU G 452	36.413	-22.062	88.253	1.00	6.47	O
ATOM 1970	CB LEU G 452	37.411	-20.612	90.952	1.00	8.63	C
ATOM 1971	CG LEU G 452	37.922	-19.306	91.574	1.00	9.19	C
ATOM 1972	CD1 LEU G 452	39.244	-19.531	92.278	1.00	7.11	C
ATOM 1973	CD2 LEU G 452	38.097	-18.258	90.504	1.00	9.43	C
ATOM 1974	N LEU G 453	36.505	-19.847	87.892	1.00	5.67	N
ATOM 1975	CA LEU G 453	36.823	-19.944	86.475	1.00	4.79	C
ATOM 1976	C LEU G 453	38.035	-19.035	86.334	1.00	5.84	C
ATOM 1977	O LEU G 453	37.913	-17.824	86.487	1.00	5.97	O
ATOM 1978	CB LEU G 453	35.688	-19.382	85.635	1.00	4.15	C
ATOM 1979	CG LEU G 453	34.367	-20.112	85.431	1.00	3.40	C
ATOM 1980	CD1 LEU G 453	33.321	-19.110	84.932	1.00	2.00	C
ATOM 1981	CD2 LEU G 453	34.556	-21.226	84.431	1.00	4.15	C
ATOM 1982	N LEU G 454	39.206	-19.606	86.084	1.00	6.21	N
ATOM 1983	CA LEU G 454	40.424	-18.815	85.975	1.00	6.68	C
ATOM 1984	C LEU G 454	41.013	-18.696	84.571	1.00	9.91	C
ATOM 1985	O LEU G 454	40.426	-19.144	83.577	1.00	8.93	O
ATOM 1986	CB LEU G 454	41.488	-19.417	86.876	1.00	5.38	C
ATOM 1987	CG LEU G 454	41.157	-19.607	88.345	1.00	5.22	C
ATOM 1988	CD1 LEU G 454	42.155	-20.577	88.956	1.00	3.11	C
ATOM 1989	CD2 LEU G 454	41.188	-18.260	89.039	1.00	2.50	C
ATOM 1990	N THR G 455	42.212	-18.122	84.535	1.00	13.23	N
ATOM 1991	CA THR G 455	42.994	-17.909	83.328	1.00	16.95	C
ATOM 1992	C THR G 455	44.440	-17.694	83.785	1.00	20.50	C
ATOM 1993	O THR G 455	44.679	-17.180	84.883	1.00	23.09	O
ATOM 1994	CB THR G 455	42.460	-16.695	82.546	1.00	16.91	C
ATOM 1995	OG1 THR G 455	41.680	-17.158	81.434	1.00	19.13	O
ATOM 1996	CG2 THR G 455	43.585	-15.798	82.051	1.00	17.25	C
ATOM 1997	N ARG G 456	45.408	-18.091	82.967	1.00	22.71	N
ATOM 1998	CA ARG G 456	46.812	-17.943	83.354	1.00	24.43	C
ATOM 1999	C ARG G 456	47.642	-16.983	82.497	1.00	25.31	C
ATOM 2000	O ARG G 456	47.496	-16.940	81.270	1.00	25.02	O
ATOM 2001	CB ARG G 456	47.492	-19.307	83.356	1.00	24.98	C
ATOM 2002	CG ARG G 456	47.524	-19.973	81.992	1.00	27.29	C
ATOM 2003	CD ARG G 456	48.361	-21.238	81.995	1.00	26.58	C
ATOM 2004	NE ARG G 456	49.779	-20.977	82.237	1.00	26.43	N
ATOM 2005	CZ ARG G 456	50.761	-21.347	81.421	1.00	26.92	C
ATOM 2006	NH1 ARG G 456	50.484	-22.002	80.306	1.00	29.13	N
ATOM 2007	NH2 ARG G 456	52.018	-21.074	81.722	1.00	27.21	N
ATOM 2008	N ASP G 457	48.516	-16.221	83.152	1.00	26.11	N
ATOM 2009	CA ASP G 457	49.399	-15.289	82.456	1.00	27.22	C
ATOM 2010	C ASP G 457	50.363	-16.131	81.632	1.00	29.84	C
ATOM 2011	O ASP G 457	50.728	-17.246	82.031	1.00	30.22	O
ATOM 2012	CB ASP G 457	50.182	-14.417	83.453	1.00	24.42	C
ATOM 2013	CG ASP G 457	49.398	-13.195	83.925	1.00	20.39	C
ATOM 2014	OD1 ASP G 457	48.176	-13.116	83.694	1.00	17.81	O
ATOM 2015	OD2 ASP G 457	50.008	-12.292	84.529	1.00	17.85	O
ATOM 2016	N GLY G 458	50.766	-15.613	80.479	1.00	32.53	N
ATOM 2017	CA GLY G 458	51.676	-16.358	79.626	1.00	34.72	C
ATOM 2018	C GLY G 458	53.059	-15.760	79.495	1.00	35.98	C
ATOM 2019	O GLY G 458	53.524	-15.041	80.382	1.00	35.17	O
ATOM 2020	N GLY G 459	53.729	-16.104	78.397	1.00	37.74	N
ATOM 2021	CA GLY G 459	55.066	-15.602	78.135	1.00	42.30	C

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FIG. 53-37

ATOM 2023	O	GLY G 459	57.194	-15.483	79.223	1.00	45.22	O
ATOM 2024	N	ASN G 460	55.684	-16.966	80.026	1.00	48.72	N
ATOM 2025	CA	ASN G 460	56.513	-17.465	81.120	1.00	50.85	C
ATOM 2026	C	ASN G 460	56.283	-18.974	81.242	1.00	50.87	C
ATOM 2027	O	ASN G 460	56.306	-19.544	82.334	1.00	50.15	O
ATOM 2028	CB	ASN G 460	56.107	-16.757	82.419	1.00	52.45	C
ATOM 2029	CG	ASN G 460	57.030	-17.076	83.573	1.00	54.62	C
ATOM 2030	OD1	ASN G 460	58.097	-16.475	83.716	1.00	56.03	O
ATOM 2031	ND2	ASN G 460	56.636	-18.036	84.397	1.00	54.44	N
ATOM 2032	N	SER G 461	56.092	-19.619	80.096	1.00	51.32	N
ATOM 2033	CA	SER G 461	55.829	-21.051	80.038	1.00	51.66	C
ATOM 2034	C	SER G 461	56.853	-21.875	80.820	1.00	51.52	C
ATOM 2035	O	SER G 461	58.055	-21.631	80.733	1.00	51.69	O
ATOM 2036	CB	SER G 461	55.782	-21.502	78.570	1.00	52.14	C
ATOM 2037	OG	SER G 461	55.295	-22.825	78.424	1.00	50.74	O
ATOM 2038	N	ASN G 462	56.347	-22.778	81.658	1.00	51.54	N
ATOM 2039	CA	ASN G 462	57.160	-23.698	82.467	1.00	51.71	C
ATOM 2040	C	ASN G 462	58.189	-23.092	83.431	1.00	51.30	C
ATOM 2041	O	ASN G 462	58.935	-23.836	84.074	1.00	51.47	O
ATOM 2042	CB	ASN G 462	57.890	-24.706	81.567	1.00	51.79	C
ATOM 2043	CG	ASN G 462	57.045	-25.198	80.406	1.00	51.91	C
ATOM 2044	OD1	ASN G 462	56.188	-26.072	80.573	1.00	52.36	O
ATOM 2045	ND2	ASN G 462	57.299	-24.652	79.219	1.00	50.59	N
ATOM 2046	N	ASN G 463	58.238	-21.766	83.537	1.00	50.19	N
ATOM 2047	CA	ASN G 463	59.200	-21.093	84.422	1.00	47.89	C
ATOM 2048	C	ASN G 463	58.755	-21.152	85.896	1.00	45.80	C
ATOM 2049	O	ASN G 463	57.704	-21.710	86.207	1.00	46.07	O
ATOM 2050	CB	ASN G 463	59.409	-19.645	83.955	1.00	47.92	C
ATOM 2051	CG	ASN G 463	60.579	-18.960	84.642	1.00	47.51	C
ATOM 2052	OD1	ASN G 463	61.518	-19.608	85.098	1.00	46.84	O
ATOM 2053	ND2	ASN G 463	60.518	-17.638	84.727	1.00	47.03	N
ATOM 2054	N	GLU G 464	59.530	-20.553	86.794	1.00	43.03	N
ATOM 2055	CA	GLU G 464	59.227	-20.577	88.224	1.00	40.21	C
ATOM 2056	C	GLU G 464	57.888	-20.097	88.778	1.00	37.07	C
ATOM 2057	O	GLU G 464	57.454	-20.582	89.825	1.00	37.50	O
ATOM 2058	CB	GLU G 464	60.374	-19.953	89.021	1.00	40.87	C
ATOM 2059	CG	GLU G 464	61.668	-20.741	88.900	1.00	41.67	C
ATOM 2060	CD	GLU G 464	61.450	-22.230	89.078	1.00	41.03	C
ATOM 2061	OE1	GLU G 464	61.274	-22.671	90.235	1.00	42.50	O
ATOM 2062	OE2	GLU G 464	61.423	-22.952	88.058	1.00	39.27	O
ATOM 2063	N	SER G 465	57.216	-19.175	88.102	1.00	32.54	N
ATOM 2064	CA	SER G 465	55.935	-18.693	88.618	1.00	29.12	C
ATOM 2065	C	SER G 465	54.817	-18.762	87.595	1.00	26.81	C
ATOM 2066	O	SER G 465	55.070	-18.752	86.395	1.00	27.05	O
ATOM 2067	CB	SER G 465	56.060	-17.259	89.136	1.00	28.35	C
ATOM 2068	OG	SER G 465	56.650	-17.216	90.426	1.00	27.82	O
ATOM 2069	N	GLU G 466	53.582	-18.846	88.076	1.00	24.12	N
ATOM 2070	CA	GLU G 466	52.421	-18.895	87.202	1.00	23.43	C
ATOM 2071	C	GLU G 466	51.353	-18.009	87.817	1.00	22.73	C
ATOM 2072	O	GLU G 466	50.918	-18.254	88.935	1.00	22.13	O
ATOM 2073	CB	GLU G 466	51.883	-20.320	87.071	1.00	25.08	C
ATOM 2074	CG	GLU G 466	52.819	-21.325	86.405	1.00	27.43	C
ATOM 2075	CD	GLU G 466	53.174	-20.957	84.981	1.00	27.92	C
ATOM 2076	OE1	GLU G 466	52.354	-20.282	84.319	1.00	27.68	O
ATOM 2077	OE2	GLU G 466	54.269	-21.363	84.522	1.00	27.89	O
ATOM 2078	N	ILE G 467	50.970	-16.954	87.104	1.00	21.51	N
ATOM 2079	CA	ILE G 467	49.956	-16.027	87.581	1.00	19.59	C
ATOM 2080	C	ILE G 467	48.600	-16.506	87.084	1.00	18.09	C
ATOM 2081	O	ILE G 467	48.475	-16.904	85.925	1.00	19.05	O
ATOM 2082	CB	ILE G 467	50.195	-14.589	87.053	1.00	20.01	C
ATOM 2083	CG1	ILE G 467	51.511	-14.014	87.596	1.00	21.88	C
ATOM 2084	CG2	ILE G 467	49.039	-13.678	87.465	1.00	18.52	C
ATOM 2085	CD1	ILE G 467	52.770	-14.461	86.849	1.00	23.23	C
ATOM 2086	N	PHE G 468	47.593	-16.469	87.957	1.00	15.14	N
ATOM 2087	CA	PHE G 468	46.239	-16.888	87.605	1.00	11.77	C
ATOM 2088	C	PHE G 468	45.268	-15.798	87.991	1.00	11.15	C
ATOM 2089	O	PHE G 468	45.252	-15.355	89.141	1.00	11.64	O
ATOM 2090	CB	PHE G 468	45.855	-18.167	88.343	1.00	9.01	C
ATOM 2091	CG	PHE G 468	46.752	-19.319	88.044	1.00	8.15	C
ATOM 2092	CD1	PHE G 468	47.923	-19.499	88.766	1.00	4.60	C

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FIG. 53-38

ATOM 2094	CE1 PHE G 468	48.785	-20.535	88.460	1.00	5.10	C
ATOM 2095	CE2 PHE G 468	47.318	-21.242	86.695	1.00	6.47	C
ATOM 2096	CZ PHE G 468	48.487	-21.406	87.424	1.00	5.03	C
ATOM 2097	N ARG G 469	44.448	-15.376	87.043	1.00	10.23	N
ATOM 2098	CA ARG G 469	43.470	-14.326	87.311	1.00	10.26	C
ATOM 2099	C ARG G 469	42.069	-14.862	87.094	1.00	8.75	C
ATOM 2100	O ARG G 469	41.874	-15.834	86.377	1.00	9.27	O
ATOM 2101	CB ARG G 469	43.691	-13.141	86.365	1.00	8.59	C
ATOM 2102	CG ARG G 469	45.117	-12.665	86.292	1.00	8.69	C
ATOM 2103	CD ARG G 469	45.258	-11.600	85.246	1.00	10.54	C
ATOM 2104	NE ARG G 469	46.654	-11.230	85.027	1.00	12.67	N
ATOM 2105	CZ ARG G 469	47.195	-10.061	85.360	1.00	11.60	C
ATOM 2106	NH1 ARG G 469	46.466	-9.122	85.953	1.00	9.15	N
ATOM 2107	NH2 ARG G 469	48.462	-9.829	85.061	1.00	13.57	N
ATOM 2108	N PRO G 470	41.076	-14.233	87.721	1.00	8.09	N
ATOM 2109	CA PRO G 470	39.682	-14.644	87.584	1.00	9.26	C
ATOM 2110	C PRO G 470	39.227	-14.487	86.129	1.00	9.58	C
ATOM 2111	O PRO G 470	39.766	-13.656	85.379	1.00	10.54	O
ATOM 2112	CB PRO G 470	38.956	-13.658	88.490	1.00	11.72	C
ATOM 2113	CG PRO G 470	39.816	-12.447	88.418	1.00	10.44	C
ATOM 2114	CD PRO G 470	41.178	-13.047	88.579	1.00	9.29	C
ATOM 2115	N GLY G 471	38.197	-15.233	85.749	1.00	6.90	N
ATOM 2116	CA GLY G 471	37.719	-15.171	84.382	1.00	3.74	C
ATOM 2117	C GLY G 471	36.224	-15.326	84.324	1.00	3.27	C
ATOM 2118	O GLY G 471	35.517	-15.032	85.280	1.00	3.93	O
ATOM 2119	N GLY G 472	35.742	-15.828	83.203	1.00	4.03	N
ATOM 2120	CA GLY G 472	34.317	-16.007	83.032	1.00	5.04	C
ATOM 2121	C GLY G 472	33.908	-15.225	81.807	1.00	5.06	C
ATOM 2122	O GLY G 472	34.739	-14.576	81.167	1.00	5.90	O
ATOM 2123	N GLY G 473	32.629	-15.267	81.481	1.00	5.75	N
ATOM 2124	CA GLY G 473	32.158	-14.548	80.312	1.00	8.01	C
ATOM 2125	C GLY G 473	31.368	-15.484	79.429	1.00	8.42	C
ATOM 2126	O GLY G 473	30.239	-15.171	79.032	1.00	8.69	O
ATOM 2127	N ASP G 474	31.958	-16.630	79.109	1.00	8.01	N
ATOM 2128	CA ASP G 474	31.248	-17.588	78.287	1.00	10.05	C
ATOM 2129	C ASP G 474	30.379	-18.349	79.262	1.00	10.61	C
ATOM 2130	O ASP G 474	30.880	-19.102	80.092	1.00	11.51	O
ATOM 2131	CB ASP G 474	32.211	-18.536	77.569	1.00	12.12	C
ATOM 2132	CG ASP G 474	31.530	-19.324	76.444	1.00	15.87	C
ATOM 2133	OD1 ASP G 474	30.274	-19.380	76.408	1.00	15.73	O
ATOM 2134	OD2 ASP G 474	32.248	-19.870	75.573	1.00	17.45	O
ATOM 2135	N MET G 475	29.082	-18.087	79.236	1.00	10.97	N
ATOM 2136	CA MET G 475	28.185	-18.779	80.148	1.00	12.17	C
ATOM 2137	C MET G 475	28.191	-20.282	79.883	1.00	11.60	C
ATOM 2138	O MET G 475	27.747	-21.067	80.726	1.00	12.20	O
ATOM 2139	CB MET G 475	26.774	-18.209	80.056	1.00	14.44	C
ATOM 2140	CG MET G 475	26.231	-17.736	81.395	1.00	15.72	C
ATOM 2141	SD MET G 475	27.411	-16.723	82.311	1.00	17.42	S
ATOM 2142	CE MET G 475	27.326	-15.188	81.444	1.00	16.54	C
ATOM 2143	N ARG G 476	28.716	-20.684	78.725	1.00	11.20	N
ATOM 2144	CA ARG G 476	28.808	-22.097	78.377	1.00	8.61	C
ATOM 2145	C ARG G 476	29.737	-22.729	79.392	1.00	7.65	C
ATOM 2146	O ARG G 476	29.467	-23.809	79.902	1.00	8.65	O
ATOM 2147	CB ARG G 476	29.375	-22.285	76.970	1.00	8.85	C
ATOM 2148	CG ARG G 476	28.434	-21.940	75.854	1.00	7.46	C
ATOM 2149	CD ARG G 476	29.093	-22.121	74.504	1.00	10.82	C
ATOM 2150	NE ARG G 476	28.198	-21.721	73.417	1.00	16.50	N
ATOM 2151	CZ ARG G 476	27.968	-20.457	73.051	1.00	18.86	C
ATOM 2152	NH1 ARG G 476	28.580	-19.452	73.682	1.00	19.84	N
ATOM 2153	NH2 ARG G 476	27.090	-20.195	72.085	1.00	18.06	N
ATOM 2154	N ASP G 477	30.809	-22.024	79.730	1.00	7.09	N
ATOM 2155	CA ASP G 477	31.766	-22.520	80.710	1.00	7.45	C
ATOM 2156	C ASP G 477	31.134	-22.709	82.105	1.00	7.05	C
ATOM 2157	O ASP G 477	31.748	-23.292	82.999	1.00	8.82	O
ATOM 2158	CB ASP G 477	32.970	-21.583	80.787	1.00	7.33	C
ATOM 2159	CG ASP G 477	33.951	-21.790	79.650	1.00	9.77	C
ATOM 2160	OD1 ASP G 477	33.775	-22.741	78.852	1.00	11.46	O
ATOM 2161	OD2 ASP G 477	34.928	-21.010	79.565	1.00	10.97	O
ATOM 2162	N ASN G 478	29.914	-22.207	82.276	1.00	6.21	N
ATOM 2163	CA ASN G 478	29.156	-22.313	83.522	1.00	7.08	C

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FIG. 53-39	ATOM 2165	O ASN G 478	28.013 -24.195	84.510	1.00	8.61	O
	ATOM 2166	CB ASN G 478	28.226 -21.106	83.679	1.00	6.30	C
	ATOM 2167	CG ASN G 478	28.946 -19.851	84.155	1.00	6.66	C
	ATOM 2168	OD1 ASN G 478	28.388 -19.083	84.941	1.00	6.95	O
	ATOM 2169	ND2 ASN G 478	30.181 -19.638	83.692	1.00	2.00	N
	ATOM 2170	N TRP G 479	27.822 -23.918	82.288	1.00	10.60	N
	ATOM 2171	CA TRP G 479	27.021 -25.117	82.112	1.00	10.15	C
	ATOM 2172	C TRP G 479	27.982 -26.318	82.084	1.00	10.73	C
	ATOM 2173	O TRP G 479	27.695 -27.380	82.620	1.00	10.51	O
	ATOM 2174	CB TRP G 479	26.241 -25.049	80.799	1.00	9.36	C
	ATOM 2175	CG TRP G 479	25.553 -23.727	80.471	1.00	9.36	C
	ATOM 2176	CD1 TRP G 479	25.260 -23.253	79.217	1.00	8.73	C
	ATOM 2177	CD2 TRP G 479	25.058 -22.734	81.390	1.00	10.20	C
	ATOM 2178	NE1 TRP G 479	24.622 -22.041	79.300	1.00	8.27	N
	ATOM 2179	CE2 TRP G 479	24.481 -21.698	80.617	1.00	9.64	C
	ATOM 2180	CE3 TRP G 479	25.043 -22.618	82.789	1.00	8.56	C
	ATOM 2181	CZ2 TRP G 479	23.897 -20.566	81.197	1.00	9.67	C
	ATOM 2182	CZ3 TRP G 479	24.461 -21.488	83.362	1.00	6.16	C
	ATOM 2183	CH2 TRP G 479	23.896 -20.481	82.566	1.00	5.85	C
	ATOM 2184	N ARG G 480	29.147 -26.117	81.484	1.00	12.12	N
	ATOM 2185	CA ARG G 480	30.182 -27.140	81.354	1.00	12.92	C
	ATOM 2186	C ARG G 480	30.630 -27.739	82.686	1.00	11.60	C
	ATOM 2187	O ARG G 480	30.971 -28.916	82.753	1.00	12.61	O
	ATOM 2188	CB ARG G 480	31.386 -26.537	80.631	1.00	16.02	C
	ATOM 2189	CG ARG G 480	32.292 -27.541	79.958	1.00	20.91	C
	ATOM 2190	CD ARG G 480	33.048 -26.879	78.815	1.00	23.41	C
	ATOM 2191	NE ARG G 480	32.155 -26.451	77.746	1.00	27.66	N
	ATOM 2192	CZ ARG G 480	32.484 -25.573	76.800	1.00	30.70	C
	ATOM 2193	NH1 ARG G 480	33.691 -25.022	76.792	1.00	33.79	N
	ATOM 2194	NH2 ARG G 480	31.604 -25.258	75.852	1.00	32.11	N
	ATOM 2195	N SER G 481	30.640 -26.926	83.738	1.00	10.12	N
	ATOM 2196	CA SER G 481	31.049 -27.368	85.069	1.00	8.15	C
	ATOM 2197	C SER G 481	30.074 -28.352	85.710	1.00	9.80	C
	ATOM 2198	O SER G 481	30.440 -29.100	86.620	1.00	10.81	O
	ATOM 2199	CB SER G 481	31.212 -26.154	85.983	1.00	7.90	C
	ATOM 2200	OG SER G 481	30.037 -25.365	86.021	1.00	3.17	O
	ATOM 2201	N GLU G 482	28.825 -28.311	85.262	1.00	11.73	N
	ATOM 2202	CA GLU G 482	27.767 -29.187	85.764	1.00	13.27	C
	ATOM 2203	C GLU G 482	27.511 -30.380	84.841	1.00	11.63	C
	ATOM 2204	O GLU G 482	27.159 -31.467	85.295	1.00	11.49	O
	ATOM 2205	CB GLU G 482	26.465 -28.395	85.923	1.00	15.44	C
	ATOM 2206	CG GLU G 482	26.389 -27.534	87.168	1.00	18.18	C
	ATOM 2207	CD GLU G 482	26.027 -28.317	88.421	1.00	20.60	C
	ATOM 2208	OE1 GLU G 482	26.223 -29.552	88.450	1.00	22.73	O
	ATOM 2209	OE2 GLU G 482	25.543 -27.694	89.389	1.00	19.58	O
	ATOM 2210	N LEU G 483	27.707 -30.169	83.547	1.00	10.75	N
	ATOM 2211	CA LEU G 483	27.473 -31.197	82.540	1.00	12.96	C
	ATOM 2212	C LEU G 483	28.697 -32.002	82.100	1.00	14.52	C
	ATOM 2213	O LEU G 483	28.565 -32.925	81.310	1.00	15.31	O
	ATOM 2214	CB LEU G 483	26.822 -30.562	81.308	1.00	11.55	C
	ATOM 2215	CG LEU G 483	25.442 -29.946	81.546	1.00	13.17	C
	ATOM 2216	CD1 LEU G 483	25.059 -29.037	80.396	1.00	13.84	C
	ATOM 2217	CD2 LEU G 483	24.413 -31.042	81.734	1.00	14.83	C
	ATOM 2218	N TYR G 484	29.871 -31.692	82.637	1.00	16.23	N
	ATOM 2219	CA TYR G 484	31.097 -32.394	82.261	1.00	17.00	C
	ATOM 2220	C TYR G 484	30.984 -33.923	82.234	1.00	17.95	C
	ATOM 2221	O TYR G 484	31.395 -34.571	81.274	1.00	20.37	O
	ATOM 2222	CB TYR G 484	32.254 -31.985	83.187	1.00	15.95	C
	ATOM 2223	CG TYR G 484	32.069 -32.445	84.615	1.00	15.50	C
	ATOM 2224	CD1 TYR G 484	31.191 -31.785	85.470	1.00	15.36	C
	ATOM 2225	CD2 TYR G 484	32.720 -33.580	85.091	1.00	13.89	C
	ATOM 2226	CE1 TYR G 484	30.954 -32.245	86.757	1.00	14.83	C
	ATOM 2227	CE2 TYR G 484	32.494 -34.047	86.375	1.00	14.19	C
	ATOM 2228	CZ TYR G 484	31.608 -33.378	87.204	1.00	14.52	C
	ATOM 2229	OH TYR G 484	31.363 -33.858	88.469	1.00	15.36	O
	ATOM 2230	N LYS G 485	30.375 -34.485	83.268	1.00	17.99	N
	ATOM 2231	CA LYS G 485	30.242 -35.929	83.409	1.00	17.32	C
	ATOM 2232	C LYS G 485	29.132 -36.579	82.592	1.00	17.71	C
	ATOM 2233	O LYS G 485	28.823 -37.755	82.805	1.00	17.90	O
	ATOM 2234	CB LYS G 485	30.030 -36.263	84.886	1.00	17.90	C



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FIG. 53-40

ATOM 2236	CD LYS G 485	28.630 -35.946 86.953 1.00 23.44	C
ATOM 2237	CE LYS G 485	27.333 -35.384 87.511 1.00 24.11	C
ATOM 2238	NZ LYS G 485	27.363 -35.232 88.997 1.00 27.95	N
ATOM 2239	N TYR G 486	28.543 -35.841 81.659 1.00 17.11	N
ATOM 2240	CA TYR G 486	27.447 -36.366 80.857 1.00 17.88	C
ATOM 2241	C TYR G 486	27.750 -36.388 79.377 1.00 19.48	C
ATOM 2242	O TYR G 486	28.700 -35.750 78.925 1.00 20.91	O
ATOM 2243	CB TYR G 486	26.196 -35.536 81.103 1.00 17.29	C
ATOM 2244	CG TYR G 486	25.733 -35.593 82.534 1.00 17.41	C
ATOM 2245	CD1 TYR G 486	25.207 -36.770 83.058 1.00 17.47	C
ATOM 2246	CD2 TYR G 486	25.823 -34.479 83.368 1.00 17.17	C
ATOM 2247	CE1 TYR G 486	24.798 -36.844 84.371 1.00 17.71	C
ATOM 2248	CE2 TYR G 486	25.412 -34.545 84.688 1.00 17.80	C
ATOM 2249	CZ TYR G 486	24.890 -35.733 85.182 1.00 16.96	C
ATOM 2250	OH TYR G 486	24.426 -35.824 86.474 1.00 18.30	O
ATOM 2251	N LYS G 487	26.956 -37.153 78.633 1.00 21.02	N
ATOM 2252	CA LYS G 487	27.107 -37.270 77.183 1.00 22.41	C
ATOM 2253	C LYS G 487	25.876 -37.937 76.587 1.00 22.55	C
ATOM 2254	O LYS G 487	25.287 -38.846 77.186 1.00 23.00	O
ATOM 2255	CB LYS G 487	28.355 -38.079 76.802 1.00 22.79	C
ATOM 2256	CG LYS G 487	28.218 -39.580 76.982 1.00 24.83	C
ATOM 2257	CD LYS G 487	29.353 -40.349 76.297 1.00 26.69	C
ATOM 2258	CE LYS G 487	29.241 -40.309 74.780 1.00 27.37	C
ATOM 2259	NZ LYS G 487	30.397 -40.984 74.131 1.00 27.40	N
ATOM 2260	N VAL G 488	25.507 -37.499 75.393 1.00 22.37	N
ATOM 2261	CA VAL G 488	24.352 -38.047 74.705 1.00 21.76	C
ATOM 2262	C VAL G 488	24.815 -39.007 73.602 1.00 22.79	C
ATOM 2263	O VAL G 488	25.655 -38.660 72.765 1.00 22.14	O
ATOM 2264	CB VAL G 488	23.444 -36.889 74.179 1.00 19.90	C
ATOM 2265	CG1 VAL G 488	23.652 -36.617 72.700 1.00 19.39	C
ATOM 2266	CG2 VAL G 488	22.007 -37.165 74.506 1.00 18.16	C
ATOM 2267	N VAL G 489	24.348 -40.245 73.673 1.00 24.24	N
ATOM 2268	CA VAL G 489	24.711 -41.265 72.687 1.00 26.29	C
ATOM 2269	C VAL G 489	23.457 -41.685 71.927 1.00 28.45	C
ATOM 2270	O VAL G 489	22.369 -41.759 72.504 1.00 29.28	O
ATOM 2271	CB VAL G 489	25.363 -42.514 73.366 1.00 25.74	C
ATOM 2272	CG1 VAL G 489	24.332 -43.315 74.152 1.00 22.14	C
ATOM 2273	CG2 VAL G 489	26.054 -43.389 72.331 1.00 26.00	C
ATOM 2274	N LYS G 490	23.588 -41.927 70.629 1.00 29.96	N
ATOM 2275	CA LYS G 490	22.431 -42.332 69.847 1.00 31.93	C
ATOM 2276	C LYS G 490	22.016 -43.753 70.218 1.00 34.03	C
ATOM 2277	O LYS G 490	22.850 -44.658 70.278 1.00 34.54	O
ATOM 2278	CB LYS G 490	22.704 -42.201 68.349 1.00 31.93	C
ATOM 2279	CG LYS G 490	21.465 -41.801 67.567 1.00 35.32	C
ATOM 2280	CD LYS G 490	21.785 -41.220 66.192 1.00 37.39	C
ATOM 2281	CE LYS G 490	20.529 -40.639 65.533 1.00 37.54	C
ATOM 2282	NZ LYS G 490	20.748 -40.207 64.118 1.00 38.65	N
ATOM 2283	N ILE G 491	20.734 -43.906 70.545 1.00 36.33	N
ATOM 2284	CA ILE G 491	20.129 -45.181 70.930 1.00 37.72	C
ATOM 2285	C ILE G 491	19.118 -45.588 69.858 1.00 39.67	C
ATOM 2286	O ILE G 491	18.473 -44.723 69.255 1.00 39.78	O
ATOM 2287	CB ILE G 491	19.406 -45.038 72.297 1.00 36.36	C
ATOM 2288	CG1 ILE G 491	20.305 -45.522 73.430 1.00 36.68	C
ATOM 2289	CG2 ILE G 491	18.075 -45.773 72.304 1.00 36.36	C
ATOM 2290	CD1 ILE G 491	20.469 -47.033 73.500 1.00 38.02	C
ATOM 2291	N GLU G 492	19.004 -46.891 69.601 1.00 41.78	N
ATOM 2292	CA GLU G 492	18.060 -47.413 68.611 1.00 43.82	C
ATOM 2293	C GLU G 492	16.694 -47.697 69.252 1.00 45.10	C
ATOM 2294	O GLU G 492	15.761 -46.903 69.003 1.00 45.64	O
ATOM 2295	CB GLU G 492	18.615 -48.676 67.940 1.00 44.12	C
ATOM 2296	CG GLU G 492	19.829 -48.437 67.043 1.00 46.18	C
ATOM 2297	CD GLU G 492	20.457 -49.729 66.524 1.00 47.97	C
ATOM 2298	OE1 GLU G 492	19.897 -50.348 65.588 1.00 47.56	O
ATOM 2299	OE2 GLU G 492	21.529 -50.112 67.042 1.00 49.02	O
ATOM 2300	OXT GLU G 492	16.573 -48.673 70.027 1.00 45.10	O
TER 2301	GLU G 492		
HETATM 2302	C1 NAG G 697	20.555 -6.134 59.155 1.00 59.64	C
HETATM 2303	C2 NAG G 697	19.931 -7.521 59.386 1.00 60.12	C
HETATM 2304	C3 NAG G 697	20.278 -8.417 58.201 1.00 59.51	C
HETATM 2305	C4 NAG G 697	19.721 -7.772 56.934 1.00 59.36	C

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FIG. 53-41	HETATM 2307	C6	NAG G 697	19.872	-5.633	55.538	1.00	60.21	C
	HETATM 2308	C7	NAG G 697	19.627	-8.793	61.463	1.00	60.60	C
	HETATM 2309	C8	NAG G 697	20.341	-9.325	62.699	1.00	59.35	C
	HETATM 2310	N2	NAG G 697	20.413	-8.118	60.621	1.00	61.24	N
	HETATM 2311	O3	NAG G 697	19.735	-9.718	58.380	1.00	58.83	O
	HETATM 2312	O4	NAG G 697	20.000	-8.588	55.801	1.00	59.07	O
	HETATM 2313	O5	NAG G 697	20.074	-5.567	57.924	1.00	59.41	O
	HETATM 2314	O6	NAG G 697	18.475	-5.375	55.596	1.00	60.26	O
	HETATM 2315	O7	NAG G 697	18.419	-8.955	61.273	1.00	59.25	O
	HETATM 2316	C1	NAG G 734	42.125	-35.659	83.656	1.00	51.27	C
	HETATM 2317	C2	NAG G 734	43.126	-36.498	84.440	1.00	53.64	C
	HETATM 2318	C3	NAG G 734	44.520	-35.939	84.253	1.00	53.54	C
	HETATM 2319	C4	NAG G 734	44.872	-35.991	82.769	1.00	52.32	C
	HETATM 2320	C5	NAG G 734	43.799	-35.348	81.871	1.00	51.37	C
	HETATM 2321	C6	NAG G 734	43.982	-35.804	80.439	1.00	49.85	C
	HETATM 2322	C7	NAG G 734	42.980	-35.689	86.776	1.00	56.96	C
	HETATM 2323	C8	NAG G 734	42.506	-36.091	88.159	1.00	57.39	C
	HETATM 2324	N2	NAG G 734	42.770	-36.622	85.845	1.00	56.31	N
	HETATM 2325	O3	NAG G 734	45.443	-36.720	84.998	1.00	54.53	O
	HETATM 2326	O4	NAG G 734	46.100	-35.311	82.562	1.00	50.81	O
	HETATM 2327	O5	NAG G 734	42.438	-35.744	82.248	1.00	50.85	O
	HETATM 2328	O6	NAG G 734	43.903	-37.244	80.404	1.00	49.02	O
	HETATM 2329	O7	NAG G 734	43.497	-34.596	86.541	1.00	57.93	O
	HETATM 2330	C1	NAG G 762	21.130	-19.832	94.879	1.00	20.43	C
	HETATM 2331	C2	NAG G 762	20.570	-19.167	96.139	1.00	22.02	C
	HETATM 2332	C3	NAG G 762	19.815	-17.879	95.806	1.00	23.32	C
	HETATM 2333	C4	NAG G 762	20.663	-16.976	94.933	1.00	24.20	C
	HETATM 2334	C5	NAG G 762	21.004	-17.767	93.674	1.00	24.06	C
	HETATM 2335	C6	NAG G 762	21.722	-16.987	92.586	1.00	21.85	C
	HETATM 2336	C7	NAG G 762	20.025	-21.017	97.650	1.00	28.11	C
	HETATM 2337	C8	NAG G 762	18.892	-21.870	98.197	1.00	28.87	C
	HETATM 2338	N2	NAG G 762	19.647	-20.087	96.780	1.00	25.44	N
	HETATM 2339	O3	NAG G 762	19.462	-17.195	96.994	1.00	23.53	O
	HETATM 2340	O4	NAG G 762	19.936	-15.797	94.615	1.00	25.52	O
	HETATM 2341	O5	NAG G 762	21.828	-18.891	94.044	1.00	24.01	O
	HETATM 2342	O6	NAG G 762	22.927	-16.416	93.070	1.00	22.76	O
	HETATM 2343	O7	NAG G 762	21.197	-21.180	97.986	1.00	29.82	O
	HETATM 2344	C1	NAG G 776	47.194	-26.706	72.904	1.00	29.03	C
	HETATM 2345	C2	NAG G 776	46.843	-26.624	71.420	1.00	28.27	C
	HETATM 2346	C3	NAG G 776	47.591	-25.464	70.776	1.00	29.77	C
	HETATM 2347	C4	NAG G 776	49.045	-25.425	71.270	1.00	30.66	C
	HETATM 2348	C5	NAG G 776	49.103	-25.289	72.793	1.00	30.69	C
	HETATM 2349	C6	NAG G 776	49.612	-23.936	73.245	1.00	31.96	C
	HETATM 2350	C7	NAG G 776	46.445	-28.953	70.822	1.00	26.40	C
	HETATM 2351	C8	NAG G 776	47.020	-30.157	70.096	1.00	27.26	C
	HETATM 2352	N2	NAG G 776	47.212	-27.870	70.777	1.00	26.77	N
	HETATM 2353	O3	NAG G 776	46.933	-24.240	71.085	1.00	32.45	O
	HETATM 2354	O4	NAG G 776	49.713	-26.616	70.881	1.00	31.22	O
	HETATM 2355	O5	NAG G 776	47.785	-25.480	73.353	1.00	30.33	O
	HETATM 2356	O6	NAG G 776	48.972	-22.885	72.538	1.00	34.50	O
	HETATM 2357	O7	NAG G 776	45.350	-28.970	71.381	1.00	25.78	O
	HETATM 2358	C1	NAG G 789	39.622	-31.812	99.985	1.00	33.09	C
	HETATM 2359	C2	NAG G 789	41.091	-31.595	100.379	1.00	35.79	C
	HETATM 2360	C3	NAG G 789	41.464	-32.456	101.583	1.00	38.23	C
	HETATM 2361	C4	NAG G 789	40.468	-32.287	102.728	1.00	38.02	C
	HETATM 2362	C5	NAG G 789	39.027	-32.466	102.205	1.00	37.00	C
	HETATM 2363	C6	NAG G 789	37.964	-32.196	103.263	1.00	36.92	C
	HETATM 2364	C7	NAG G 789	42.221	-31.188	98.239	1.00	38.71	C
	HETATM 2365	C8	NAG G 789	43.194	-31.796	97.241	1.00	38.54	C
	HETATM 2366	N2	NAG G 789	41.974	-31.962	99.288	1.00	36.82	N
	HETATM 2367	O3	NAG G 789	42.771	-32.119	102.028	1.00	40.34	O
	HETATM 2368	O4	NAG G 789	40.753	-33.260	103.734	1.00	36.57	O
	HETATM 2369	O5	NAG G 789	38.776	-31.559	101.110	1.00	33.56	O
	HETATM 2370	O6	NAG G 789	36.661	-32.387	102.737	1.00	34.73	O
	HETATM 2371	O7	NAG G 789	41.692	-30.092	98.076	1.00	40.67	O
	HETATM 2372	C1	NAG G 795	26.343	-15.597	105.566	1.00	33.85	C
	HETATM 2373	C2	NAG G 795	27.454	-15.427	106.588	1.00	34.59	C
	HETATM 2374	C3	NAG G 795	27.804	-16.830	107.085	1.00	33.53	C
	HETATM 2375	C4	NAG G 795	26.576	-17.377	107.789	1.00	34.67	C
	HETATM 2376	C5	NAG G 795	25.361	-17.390	106.844	1.00	35.20	C

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FIG. 53-42	HETATM 2378	C7	NAG G 795	29.721	-15.240	105.605	1.00	35.20	C
	HETATM 2379	C8	NAG G 795	30.722	-14.216	105.110	1.00	33.50	C
	HETATM 2380	N2	NAG G 795	28.585	-14.693	106.045	1.00	34.80	N
	HETATM 2381	O3	NAG G 795	28.901	-16.798	107.984	1.00	31.29	O
	HETATM 2382	O4	NAG G 795	26.838	-18.693	108.266	1.00	36.45	O
	HETATM 2383	O5	NAG G 795	25.164	-16.082	106.229	1.00	34.33	O
	HETATM 2384	O6	NAG G 795	22.929	-17.316	106.880	1.00	37.82	O
	HETATM 2385	O7	NAG G 795	29.948	-16.455	105.616	1.00	36.36	O
	HETATM 2386	C1	NAG G 832	28.226	-9.645	104.992	1.00	45.87	C
	HETATM 2387	C2	NAG G 832	27.974	-8.717	103.779	1.00	47.52	C
	HETATM 2388	C3	NAG G 832	26.672	-7.923	103.865	1.00	47.38	C
	HETATM 2389	C4	NAG G 832	25.536	-8.834	104.242	1.00	47.85	C
	HETATM 2390	C5	NAG G 832	25.893	-9.462	105.568	1.00	48.32	C
	HETATM 2391	C6	NAG G 832	24.771	-10.301	106.124	1.00	49.64	C
	HETATM 2392	C7	NAG G 832	29.433	-6.905	104.549	1.00	50.62	C
	HETATM 2393	C8	NAG G 832	30.638	-6.054	104.182	1.00	50.60	C
	HETATM 2394	N2	NAG G 832	29.086	-7.795	103.623	1.00	49.35	N
	HETATM 2395	O3	NAG G 832	26.389	-7.335	102.610	1.00	46.59	O
	HETATM 2396	O4	NAG G 832	24.339	-8.081	104.350	1.00	49.40	O
	HETATM 2397	O5	NAG G 832	27.025	-10.331	105.389	1.00	47.66	O
	HETATM 2398	O6	NAG G 832	24.829	-11.627	105.607	1.00	52.39	O
	HETATM 2399	O7	NAG G 832	28.806	-6.757	105.595	1.00	51.02	O
	HETATM 2400	C1	NAG G 839	45.384	-15.132	101.861	1.00	48.21	C
	HETATM 2401	C2	NAG G 839	45.794	-14.589	100.496	1.00	48.49	C
	HETATM 2402	C3	NAG G 839	44.600	-13.920	99.790	1.00	50.29	C
	HETATM 2403	C4	NAG G 839	43.333	-14.084	100.623	1.00	51.29	C
	HETATM 2404	C5	NAG G 839	43.588	-13.499	102.001	1.00	51.81	C
	HETATM 2405	C6	NAG G 839	42.436	-13.580	102.964	1.00	52.61	C
	HETATM 2406	C7	NAG G 839	46.867	-12.432	101.084	1.00	48.14	C
	HETATM 2407	C8	NAG G 839	48.204	-11.709	101.107	1.00	47.76	C
	HETATM 2408	N2	NAG G 839	46.931	-13.683	100.621	1.00	48.44	N
	HETATM 2409	O3	NAG G 839	44.391	-14.504	98.514	1.00	49.77	O
	HETATM 2410	O4	NAG G 839	42.266	-13.392	99.990	1.00	52.56	O
	HETATM 2411	O5	NAG G 839	44.717	-14.131	102.652	1.00	51.72	O
	HETATM 2412	O6	NAG G 839	42.786	-12.941	104.186	1.00	51.16	O
	HETATM 2413	O7	NAG G 839	45.824	-11.900	101.451	1.00	47.23	O
	HETATM 2414	C1	NAG G 886	38.263	-1.983	93.510	1.00	10.19	C
	HETATM 2415	C2	NAG G 886	39.603	-2.388	94.081	1.00	11.25	C
	HETATM 2416	C3	NAG G 886	40.644	-1.429	93.556	1.00	8.62	C
	HETATM 2417	C4	NAG G 886	40.684	-1.576	92.052	1.00	6.43	C
	HETATM 2418	C5	NAG G 886	39.309	-1.295	91.444	1.00	6.21	C
	HETATM 2419	C6	NAG G 886	39.275	-1.678	89.965	1.00	6.26	C
	HETATM 2420	C7	NAG G 886	39.359	-3.470	96.261	1.00	20.54	C
	HETATM 2421	C8	NAG G 886	39.345	-3.231	97.770	1.00	21.65	C
	HETATM 2422	N2	NAG G 886	39.557	-2.371	95.531	1.00	18.35	N
	HETATM 2423	O3	NAG G 886	41.918	-1.723	94.108	1.00	5.81	O
	HETATM 2424	O4	NAG G 886	41.632	-0.671	91.524	1.00	6.73	O
	HETATM 2425	O5	NAG G 886	38.286	-2.088	92.087	1.00	9.22	O
	HETATM 2426	O6	NAG G 886	37.970	-2.092	89.567	1.00	6.56	O
	HETATM 2427	O7	NAG G 886	39.224	-4.589	95.758	1.00	21.08	O
	HETATM 2428	C1	NAG G 892	46.184	-7.814	97.674	1.00	47.50	C
	HETATM 2429	C2	NAG G 892	45.528	-6.456	97.388	1.00	49.91	C
	HETATM 2430	C3	NAG G 892	44.626	-6.058	98.564	1.00	50.40	C
	HETATM 2431	C4	NAG G 892	43.661	-7.190	98.908	1.00	50.85	C
	HETATM 2432	C5	NAG G 892	44.446	-8.485	99.149	1.00	50.35	C
	HETATM 2433	C6	NAG G 892	43.620	-9.712	99.508	1.00	50.08	C
	HETATM 2434	C7	NAG G 892	46.349	-4.288	96.593	1.00	50.40	C
	HETATM 2435	C8	NAG G 892	47.573	-3.388	96.528	1.00	50.74	C
	HETATM 2436	N2	NAG G 892	46.560	-5.448	97.209	1.00	51.09	N
	HETATM 2437	O3	NAG G 892	43.880	-4.889	98.245	1.00	50.85	O
	HETATM 2438	O4	NAG G 892	42.920	-6.835	100.066	1.00	51.88	O
	HETATM 2439	O5	NAG G 892	45.198	-8.806	97.970	1.00	48.21	O
	HETATM 2440	O6	NAG G 892	42.430	-9.339	100.240	1.00	50.76	O
	HETATM 2441	O7	NAG G 892	45.259	-3.974	96.112	1.00	49.47	O
	HETATM 2442	C1	NAG G 948	25.295	-22.817	101.637	1.00	40.79	C
	HETATM 2443	C2	NAG G 948	24.518	-21.842	102.514	1.00	42.75	C
	HETATM 2444	C3	NAG G 948	24.415	-22.474	103.889	1.00	43.06	C
	HETATM 2445	C4	NAG G 948	23.648	-23.791	103.786	1.00	43.39	C
	HETATM 2446	C5	NAG G 948	24.232	-24.720	102.690	1.00	43.93	C
	HETATM 2447	C6	NAG G 948	23.250	-25.813	102.286	1.00	45.28	C

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FIG. 53-43	HETATM 2449	C8	NAG G 948	25.354	-18.157	102.738	1.00	45.91	C
	HETATM 2450	N2	NAG G 948	25.166	-20.546	102.603	1.00	44.95	N
	HETATM 2451	O3	NAG G 948	23.751	-21.592	104.775	1.00	41.16	O
	HETATM 2452	O4	NAG G 948	23.691	-24.450	105.045	1.00	44.20	O
	HETATM 2453	O5	NAG G 948	24.512	-23.997	101.459	1.00	43.27	O
	HETATM 2454	O6	NAG G 948	23.025	-26.747	103.362	1.00	45.76	O
	HETATM 2455	O7	NAG G 948	23.258	-19.349	102.552	1.00	45.87	O
	HETATM 2456	C1	FUC G 735	44.832	-37.819	79.533	1.00	49.89	C
	HETATM 2457	C2	FUC G 735	44.829	-39.335	79.729	1.00	50.29	C
	HETATM 2458	C3	FUC G 735	43.517	-39.947	79.245	1.00	49.55	C
	HETATM 2459	C4	FUC G 735	43.248	-39.510	77.810	1.00	49.76	C
	HETATM 2460	C5	FUC G 735	43.281	-37.985	77.709	1.00	51.03	C
	HETATM 2461	C6	FUC G 735	43.097	-37.486	76.286	1.00	50.15	C
	HETATM 2462	O2	FUC G 735	45.009	-39.644	81.103	1.00	51.19	O
	HETATM 2463	O3	FUC G 735	43.614	-41.363	79.303	1.00	47.91	O
	HETATM 2464	O4	FUC G 735	44.237	-40.067	76.958	1.00	48.59	O
	HETATM 2465	O5	FUC G 735	44.552	-37.492	78.179	1.00	50.30	O
	HETATM 2466	C1	FUC G 796	21.868	-18.232	106.944	1.00	39.18	C
	HETATM 2467	C2	FUC G 796	21.294	-18.306	108.369	1.00	39.82	C
	HETATM 2468	C3	FUC G 796	20.583	-16.994	108.738	1.00	40.37	C
	HETATM 2469	C4	FUC G 796	19.594	-16.548	107.660	1.00	41.30	C
	HETATM 2470	C5	FUC G 796	20.249	-16.583	106.284	1.00	41.12	C
	HETATM 2471	C6	FUC G 796	19.259	-16.299	105.170	1.00	41.28	C
	HETATM 2472	O2	FUC G 796	22.312	-18.587	109.324	1.00	36.01	O
	HETATM 2473	O3	FUC G 796	19.881	-17.154	109.963	1.00	39.31	O
	HETATM 2474	O4	FUC G 796	18.450	-17.385	107.680	1.00	41.95	O
	HETATM 2475	O5	FUC G 796	20.825	-17.887	106.043	1.00	40.79	O
	HETATM 2476	C1	FUC G 893	42.567	-9.258	101.642	1.00	50.80	C
	HETATM 2477	C2	FUC G 893	41.194	-9.514	102.274	1.00	50.38	C
	HETATM 2478	C3	FUC G 893	41.299	-10.170	103.654	1.00	49.12	C
	HETATM 2479	C4	FUC G 893	42.554	-9.716	104.378	1.00	49.68	C
	HETATM 2480	C5	FUC G 893	43.820	-10.036	103.564	1.00	50.81	C
	HETATM 2481	C6	FUC G 893	44.916	-8.991	103.707	1.00	50.38	C
	HETATM 2482	O2	FUC G 893	40.434	-10.355	101.418	1.00	50.40	O
	HETATM 2483	O3	FUC G 893	40.158	-9.815	104.427	1.00	46.21	O
	HETATM 2484	O4	FUC G 893	42.469	-8.324	104.642	1.00	50.60	O
	HETATM 2485	O5	FUC G 893	43.519	-10.180	102.153	1.00	50.37	O
	HETATM 2486	C1	FUC G 949	21.703	-26.733	103.844	1.00	48.86	C
	HETATM 2487	C2	FUC G 949	20.695	-27.189	102.761	1.00	49.59	C
	HETATM 2488	C3	FUC G 949	20.209	-28.600	103.072	1.00	50.21	C
	HETATM 2489	C4	FUC G 949	19.428	-28.569	104.380	1.00	50.60	C
	HETATM 2490	C5	FUC G 949	20.207	-27.783	105.445	1.00	51.10	C
	HETATM 2491	C6	FUC G 949	19.594	-26.439	105.805	1.00	50.80	C
	HETATM 2492	O2	FUC G 949	21.259	-27.160	101.459	1.00	49.78	O
	HETATM 2493	O3	FUC G 949	19.372	-29.064	102.021	1.00	50.49	O
	HETATM 2494	O4	FUC G 949	18.162	-27.963	104.155	1.00	49.46	O
	HETATM 2495	O5	FUC G 949	21.568	-27.546	105.009	1.00	49.90	O
	ATOM 2496	N	LYSC 1	52.519	-14.192	56.192	1.00	46.28	N
	ATOM 2497	CA	LYSC 1	52.501	-13.174	57.280	1.00	46.54	C
	ATOM 2498	C	LYSC 1	52.344	-11.780	56.675	1.00	45.07	C
	ATOM 2499	O	LYSC 1	53.179	-11.339	55.885	1.00	45.01	O
	ATOM 2500	CB	LYSC 1	53.779	-13.271	58.127	1.00	46.69	C
	ATOM 2501	CG	LYSC 1	54.092	-12.030	58.955	1.00	47.32	C
	ATOM 2502	CD	LYSC 1	55.232	-12.265	59.947	1.00	46.72	C
	ATOM 2503	CE	LYSC 1	56.361	-13.127	59.377	1.00	44.02	C
	ATOM 2504	NZ	LYSC 1	56.425	-14.429	60.099	1.00	42.44	N
	ATOM 2505	N	LYSC 2	51.240	-11.128	57.024	1.00	42.82	N
	ATOM 2506	CA	LYSC 2	50.914	-9.794	56.542	1.00	40.43	C
	ATOM 2507	C	LYSC 2	51.775	-8.746	57.238	1.00	38.15	C
	ATOM 2508	O	LYSC 2	52.171	-8.921	58.398	1.00	37.03	O
	ATOM 2509	CB	LYSC 2	49.436	-9.500	56.824	1.00	42.05	C
	ATOM 2510	CG	LYSC 2	48.531	-9.514	55.603	1.00	45.12	C
	ATOM 2511	CD	LYSC 2	48.547	-8.172	54.888	1.00	48.62	C
	ATOM 2512	CE	LYSC 2	48.042	-7.054	55.805	1.00	50.79	C
	ATOM 2513	NZ	LYSC 2	46.646	-7.283	56.307	1.00	52.67	N
	ATOM 2514	N	VAL C 3	52.078	-7.674	56.512	1.00	35.75	N
	ATOM 2515	CA	VAL C 3	52.865	-6.562	57.047	1.00	32.56	C
	ATOM 2516	C	VAL C 3	51.990	-5.307	57.081	1.00	29.97	C
	ATOM 2517	O	VAL C 3	51.403	-4.913	56.067	1.00	32.06	O
	ATOM 2518	CB	VAL C 3	54.173	-6.776	56.188	1.00	32.08	C

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FIG. 53-44

ATOM 2520	CG2 VAL C 3	54.979	-7.515	56.081	1.00	32.20	C
ATOM 2521	N VAL C 4	51.873	-4.705	58.253	1.00	26.84	N
ATOM 2522	CA VAL C 4	51.081	-3.499	58.422	1.00	24.56	C
ATOM 2523	C VAL C 4	51.964	-2.412	59.032	1.00	23.09	C
ATOM 2524	O VAL C 4	52.702	-2.657	59.991	1.00	23.17	O
ATOM 2525	CB VAL C 4	49.862	-3.754	59.335	1.00	25.14	C
ATOM 2526	CG1 VAL C 4	49.174	-2.440	59.688	1.00	25.88	C
ATOM 2527	CG2 VAL C 4	48.884	-4.696	58.653	1.00	24.55	C
ATOM 2528	N LEU C 5	51.930	-1.228	58.435	1.00	20.69	N
ATOM 2529	CA LEU C 5	52.713	-0.110	58.920	1.00	17.71	C
ATOM 2530	C LEU C 5	51.767	0.875	59.563	1.00	16.21	C
ATOM 2531	O LEU C 5	50.640	1.053	59.102	1.00	14.03	O
ATOM 2532	CB LEU C 5	53.452	0.571	57.771	1.00	19.17	C
ATOM 2533	CG LEU C 5	54.976	0.433	57.740	1.00	19.31	C
ATOM 2534	CD1 LEU C 5	55.349	-1.015	57.430	1.00	20.41	C
ATOM 2535	CD2 LEU C 5	55.560	1.376	56.692	1.00	17.06	C
ATOM 2536	N GLY C 6	52.237	1.502	60.635	1.00	16.84	N
ATOM 2537	CA GLY C 6	51.444	2.477	61.357	1.00	14.53	C
ATOM 2538	C GLY C 6	52.278	3.696	61.701	1.00	13.29	C
ATOM 2539	O GLY C 6	53.518	3.670	61.634	1.00	9.47	O
ATOM 2540	N LYS C 7	51.590	4.756	62.110	1.00	13.42	N
ATOM 2541	CA LYS C 7	52.228	6.017	62.456	1.00	14.70	C
ATOM 2542	C LYS C 7	52.227	6.231	63.966	1.00	15.10	C
ATOM 2543	O LYS C 7	51.268	5.875	64.644	1.00	15.26	O
ATOM 2544	CB LYS C 7	51.506	7.166	61.726	1.00	16.29	C
ATOM 2545	CG LYS C 7	51.575	7.042	60.191	1.00	17.07	C
ATOM 2546	CD LYS C 7	50.476	7.796	59.437	1.00	17.81	C
ATOM 2547	CE LYS C 7	50.659	9.310	59.449	1.00	20.57	C
ATOM 2548	NZ LYS C 7	50.313	9.923	60.770	1.00	28.17	N
ATOM 2549	N LYS C 8	53.329	6.755	64.499	1.00	17.20	N
ATOM 2550	CA LYS C 8	53.441	7.017	65.934	1.00	17.81	C
ATOM 2551	C LYS C 8	52.301	7.941	66.330	1.00	18.97	C
ATOM 2552	O LYS C 8	52.166	9.040	65.777	1.00	20.57	O
ATOM 2553	CB LYS C 8	54.782	7.686	66.265	1.00	16.85	C
ATOM 2554	CG LYS C 8	54.858	8.299	67.669	1.00	21.33	C
ATOM 2555	CD LYS C 8	56.179	9.042	67.918	1.00	25.64	C
ATOM 2556	CE LYS C 8	56.335	10.290	67.008	1.00	29.41	C
ATOM 2557	NZ LYS C 8	57.754	10.788	66.887	1.00	28.75	N
ATOM 2558	N GLY C 9	51.445	7.464	67.229	1.00	19.05	N
ATOM 2559	CA GLY C 9	50.330	8.268	67.696	1.00	17.56	C
ATOM 2560	C GLY C 9	48.969	7.980	67.102	1.00	17.59	C
ATOM 2561	O GLY C 9	47.958	8.239	67.756	1.00	16.57	O
ATOM 2562	N ASP C 10	48.923	7.437	65.888	1.00	19.01	N
ATOM 2563	CA ASP C 10	47.643	7.139	65.239	1.00	21.62	C
ATOM 2564	C ASP C 10	46.957	5.928	65.855	1.00	23.44	C
ATOM 2565	O ASP C 10	47.401	5.406	66.878	1.00	24.09	O
ATOM 2566	CB ASP C 10	47.824	6.914	63.730	1.00	22.83	C
ATOM 2567	CG ASP C 10	47.971	8.218	62.942	1.00	24.07	C
ATOM 2568	OD1 ASP C 10	47.688	9.309	63.483	1.00	25.82	O
ATOM 2569	OD2 ASP C 10	48.369	8.149	61.759	1.00	22.11	O
ATOM 2570	N THR C 11	45.879	5.479	65.217	1.00	25.01	N
ATOM 2571	CA THR C 11	45.106	4.328	65.679	1.00	25.73	C
ATOM 2572	C THR C 11	45.002	3.295	64.559	1.00	25.74	C
ATOM 2573	O THR C 11	44.371	3.541	63.526	1.00	27.41	O
ATOM 2574	CB THR C 11	43.690	4.769	66.127	1.00	25.46	C
ATOM 2575	OG1 THR C 11	43.796	5.608	67.287	1.00	24.74	O
ATOM 2576	CG2 THR C 11	42.827	3.573	66.460	1.00	25.70	C
ATOM 2577	N VAL C 12	45.634	2.148	64.759	1.00	25.59	N
ATOM 2578	CA VAL C 12	45.634	1.090	63.753	1.00	25.97	C
ATOM 2579	C VAL C 12	44.625	-0.028	64.043	1.00	26.00	C
ATOM 2580	O VAL C 12	44.258	-0.272	65.193	1.00	26.72	O
ATOM 2581	CB VAL C 12	47.063	0.485	63.592	1.00	24.36	C
ATOM 2582	CG1 VAL C 12	47.418	-0.371	64.790	1.00	25.22	C
ATOM 2583	CG2 VAL C 12	47.175	-0.312	62.312	1.00	23.23	C
ATOM 2584	N GLU C 13	44.154	-0.680	62.990	1.00	25.92	N
ATOM 2585	CA GLU C 13	43.220	-1.783	63.147	1.00	27.89	C
ATOM 2586	C GLU C 13	43.732	-3.000	62.387	1.00	28.19	C
ATOM 2587	O GLU C 13	43.845	-2.979	61.162	1.00	30.05	O
ATOM 2588	CB GLU C 13	41.816	-1.424	62.650	1.00	28.29	C
ATOM 2589	CG GLU C 13	40.854	-2.614	62.693	1.00	29.78	C

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FIG. 53-45	ATOM 2591	OE1 GLU C 13	38.709	-1.591	62.650	1.00	31.72	O
	ATOM 2592	OE2 GLU C 13	39.268	-2.846	60.934	1.00	30.92	O
	ATOM 2593	N LEU C 14	44.122	-4.028	63.127	1.00	27.86	N
	ATOM 2594	CA LEU C 14	44.607	-5.264	62.534	1.00	25.77	C
	ATOM 2595	C LEU C 14	43.350	-6.099	62.310	1.00	25.26	C
	ATOM 2596	O LEU C 14	42.456	-6.102	63.159	1.00	24.53	O
	ATOM 2597	CB LEU C 14	45.582	-5.949	63.493	1.00	25.87	C
	ATOM 2598	CG LEU C 14	46.783	-5.061	63.861	1.00	26.59	C
	ATOM 2599	CD1 LEU C 14	47.658	-5.719	64.905	1.00	26.29	C
	ATOM 2600	CD2 LEU C 14	47.592	-4.744	62.621	1.00	24.92	C
	ATOM 2601	N THR C 15	43.274	-6.770	61.160	1.00	25.71	N
	ATOM 2602	CA THR C 15	42.113	-7.583	60.774	1.00	24.95	C
	ATOM 2603	C THR C 15	42.204	-9.088	61.074	1.00	24.16	C
	ATOM 2604	O THR C 15	43.286	-9.686	61.056	1.00	22.82	O
	ATOM 2605	CB THR C 15	41.802	-7.413	59.257	1.00	24.70	C
	ATOM 2606	OG1 THR C 15	42.537	-6.299	58.736	1.00	23.44	O
	ATOM 2607	CG2 THR C 15	40.314	-7.166	59.037	1.00	24.46	C
	ATOM 2608	N CYS C 16	41.042	-9.690	61.317	1.00	23.58	N
	ATOM 2609	CA CYS C 16	40.943	-11.117	61.596	1.00	24.66	C
	ATOM 2610	C CYS C 16	39.517	-11.581	61.317	1.00	25.93	C
	ATOM 2611	O CYS C 16	38.567	-11.126	61.969	1.00	23.82	O
	ATOM 2612	CB CYS C 16	41.300	-11.415	63.046	1.00	24.59	C
	ATOM 2613	SG CYS C 16	41.474	-13.182	63.435	1.00	22.70	S
	ATOM 2614	N THR C 17	39.381	-12.482	60.346	1.00	28.46	N
	ATOM 2615	CA THR C 17	38.082	-13.008	59.955	1.00	30.73	C
	ATOM 2616	C THR C 17	38.059	-14.522	60.073	1.00	31.96	C
	ATOM 2617	O THR C 17	38.757	-15.232	59.345	1.00	32.62	O
	ATOM 2618	CB THR C 17	37.716	-12.576	58.519	1.00	31.47	C
	ATOM 2619	OG1 THR C 17	37.644	-11.143	58.458	1.00	32.79	O
	ATOM 2620	CG2 THR C 17	36.376	-13.154	58.109	1.00	31.32	C
	ATOM 2621	N ALA C 18	37.258	-15.005	61.016	1.00	34.59	N
	ATOM 2622	CA ALA C 18	37.105	-16.432	61.271	1.00	37.71	C
	ATOM 2623	C ALA C 18	36.883	-17.167	59.956	1.00	39.50	C
	ATOM 2624	O ALA C 18	36.149	-16.676	59.094	1.00	38.11	O
	ATOM 2625	CB ALA C 18	35.918	-16.666	62.211	1.00	37.31	C
	ATOM 2626	N SER C 19	37.537	-18.319	59.802	1.00	42.72	N
	ATOM 2627	CA SER C 19	37.423	-19.142	58.587	1.00	45.98	C
	ATOM 2628	C SER C 19	35.949	-19.410	58.282	1.00	46.99	C
	ATOM 2629	O SER C 19	35.413	-20.463	58.621	1.00	47.77	O
	ATOM 2630	CB SER C 19	38.179	-20.465	58.762	1.00	46.10	C
	ATOM 2631	OG SER C 19	38.854	-20.507	60.016	1.00	47.20	O
	ATOM 2632	N GLN C 20	35.311	-18.429	57.652	1.00	47.66	N
	ATOM 2633	CA GLN C 20	33.899	-18.460	57.315	1.00	48.47	C
	ATOM 2634	C GLN C 20	32.951	-18.862	58.434	1.00	49.07	C
	ATOM 2635	O GLN C 20	31.822	-19.313	58.211	1.00	48.95	O
	ATOM 2636	CB GLN C 20	33.644	-19.197	56.009	1.00	48.86	C
	ATOM 2637	CG GLN C 20	33.912	-18.280	54.822	1.00	50.12	C
	ATOM 2638	CD GLN C 20	33.590	-16.817	55.143	1.00	49.90	C
	ATOM 2639	OE1 GLN C 20	32.512	-16.500	55.653	1.00	48.89	O
	ATOM 2640	NE2 GLN C 20	34.539	-15.929	54.874	1.00	49.91	N
	ATOM 2641	N LYS C 21	33.394	-18.552	59.646	1.00	49.87	N
	ATOM 2642	CA LYS C 21	32.643	-18.806	60.865	1.00	49.80	C
	ATOM 2643	C LYS C 21	32.109	-17.426	61.260	1.00	49.40	C
	ATOM 2644	O LYS C 21	32.336	-16.440	60.539	1.00	49.21	O
	ATOM 2645	CB LYS C 21	33.576	-19.353	61.956	1.00	49.61	C
	ATOM 2646	CG LYS C 21	34.386	-20.576	61.548	1.00	46.89	C
	ATOM 2647	CD LYS C 21	35.843	-20.444	61.974	1.00	46.08	C
	ATOM 2648	CE LYS C 21	36.618	-21.710	61.648	1.00	47.91	C
	ATOM 2649	NZ LYS C 21	38.048	-21.682	62.078	1.00	46.72	N
	ATOM 2650	N LYS C 22	31.362	-17.356	62.360	1.00	48.20	N
	ATOM 2651	CA LYS C 22	30.802	-16.088	62.824	1.00	45.14	C
	ATOM 2652	C LYS C 22	31.290	-15.787	64.231	1.00	43.93	C
	ATOM 2653	O LYS C 22	32.382	-16.217	64.596	1.00	43.66	O
	ATOM 2654	CB LYS C 22	29.275	-16.113	62.749	1.00	42.50	C
	ATOM 2655	CG LYS C 22	28.761	-16.285	61.331	1.00	41.16	C
	ATOM 2656	CD LYS C 22	29.298	-15.185	60.430	1.00	38.60	C
	ATOM 2657	CE LYS C 22	29.385	-15.635	58.987	1.00	38.26	C
	ATOM 2658	NZ LYS C 22	30.447	-16.661	58.796	1.00	37.88	N
	ATOM 2659	N SER C 23	30.498	-15.058	65.014	1.00	42.70	N
	ATOM 2660	CA SER C 23	30.877	-14.703	66.379	1.00	42.40	C

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FIG. 53-46

ATOM	2662	O	SER	C	23	30.501	-16.619	67.785	1.00	41.43	O
ATOM	2663	CB	SER	C	23	29.721	-14.002	67.094	1.00	43.85	C
ATOM	2664	OG	SER	C	23	30.151	-13.435	68.323	1.00	45.83	O
ATOM	2665	N	ILE	C	24	32.624	-16.170	67.170	1.00	40.65	N
ATOM	2666	CA	ILE	C	24	33.211	-17.292	67.883	1.00	39.11	C
ATOM	2667	C	ILE	C	24	34.438	-16.778	68.623	1.00	37.20	C
ATOM	2668	O	ILE	C	24	34.987	-15.740	68.265	1.00	37.00	O
ATOM	2669	CB	ILE	C	24	33.622	-18.410	66.912	1.00	39.97	C
ATOM	2670	CG1	ILE	C	24	34.679	-17.899	65.928	1.00	39.87	C
ATOM	2671	CG2	ILE	C	24	32.394	-18.933	66.166	1.00	40.37	C
ATOM	2672	CD1	ILE	C	24	35.315	-18.996	65.107	1.00	39.02	C
ATOM	2673	N	GLN	C	25	34.856	-17.496	69.659	1.00	35.82	N
ATOM	2674	CA	GLN	C	25	36.010	-17.093	70.459	1.00	33.47	C
ATOM	2675	C	GLN	C	25	37.230	-16.775	69.597	1.00	30.61	C
ATOM	2676	O	GLN	C	25	37.394	-17.331	68.507	1.00	29.53	O
ATOM	2677	CB	GLN	C	25	36.355	-18.178	71.491	1.00	34.46	C
ATOM	2678	CG	GLN	C	25	36.219	-17.741	72.957	1.00	37.05	C
ATOM	2679	CD	GLN	C	25	34.773	-17.505	73.392	1.00	38.55	C
ATOM	2680	OE1	GLN	C	25	33.988	-16.890	72.673	1.00	38.36	O
ATOM	2681	NE2	GLN	C	25	34.424	-17.986	74.582	1.00	39.56	N
ATOM	2682	N	PHE	C	26	38.043	-15.837	70.075	1.00	27.82	N
ATOM	2683	CA	PHE	C	26	39.261	-15.427	69.387	1.00	25.86	C
ATOM	2684	C	PHE	C	26	40.150	-14.777	70.426	1.00	24.69	C
ATOM	2685	O	PHE	C	26	39.685	-14.460	71.523	1.00	25.10	O
ATOM	2686	CB	PHE	C	26	38.952	-14.401	68.287	1.00	24.48	C
ATOM	2687	CG	PHE	C	26	38.682	-13.009	68.807	1.00	21.65	C
ATOM	2688	CD1	PHE	C	26	37.448	-12.679	69.350	1.00	19.79	C
ATOM	2689	CD2	PHE	C	26	39.675	-12.036	68.768	1.00	19.32	C
ATOM	2690	CE1	PHE	C	26	37.206	-11.406	69.847	1.00	17.63	C
ATOM	2691	CE2	PHE	C	26	39.438	-10.763	69.265	1.00	17.64	C
ATOM	2692	CZ	PHE	C	26	38.204	-10.448	69.806	1.00	16.15	C
ATOM	2693	N	HIS	C	27	41.430	-14.617	70.095	1.00	23.03	N
ATOM	2694	CA	HIS	C	27	42.398	-13.960	70.978	1.00	21.63	C
ATOM	2695	C	HIS	C	27	43.682	-13.568	70.255	1.00	20.47	C
ATOM	2696	O	HIS	C	27	44.269	-14.373	69.526	1.00	19.01	O
ATOM	2697	CB	HIS	C	27	42.706	-14.766	72.257	1.00	22.61	C
ATOM	2698	CG	HIS	C	27	42.699	-16.257	72.074	1.00	26.73	C
ATOM	2699	ND1	HIS	C	27	43.820	-16.973	71.725	1.00	27.44	N
ATOM	2700	CD2	HIS	C	27	41.701	-17.163	72.223	1.00	28.73	C
ATOM	2701	CE1	HIS	C	27	43.516	-18.261	71.666	1.00	28.75	C
ATOM	2702	NE2	HIS	C	27	42.239	-18.400	71.962	1.00	29.75	N
ATOM	2703	N	TRP	C	28	44.048	-12.294	70.396	1.00	19.19	N
ATOM	2704	CA	TRP	C	28	45.249	-11.734	69.793	1.00	18.50	C
ATOM	2705	C	TRP	C	28	46.384	-11.806	70.810	1.00	19.12	C
ATOM	2706	O	TRP	C	28	46.189	-11.505	71.989	1.00	18.57	O
ATOM	2707	CB	TRP	C	28	45.010	-10.277	69.361	1.00	15.67	C
ATOM	2708	CG	TRP	C	28	44.134	-10.125	68.144	1.00	12.38	C
ATOM	2709	CD1	TRP	C	28	42.769	-10.196	68.098	1.00	11.68	C
ATOM	2710	CD2	TRP	C	28	44.569	-9.884	66.796	1.00	11.77	C
ATOM	2711	NE1	TRP	C	28	42.326	-10.016	66.805	1.00	11.45	N
ATOM	2712	CE2	TRP	C	28	43.408	-9.818	65.985	1.00	11.23	C
ATOM	2713	CE3	TRP	C	28	45.823	-9.718	66.185	1.00	12.46	C
ATOM	2714	CZ2	TRP	C	28	43.467	-9.592	64.603	1.00	8.94	C
ATOM	2715	CZ3	TRP	C	28	45.880	-9.497	64.806	1.00	10.11	C
ATOM	2716	CH2	TRP	C	28	44.705	-9.435	64.034	1.00	8.40	C
ATOM	2717	N	LYS	C	29	47.566	-12.190	70.336	1.00	20.29	N
ATOM	2718	CA	LYS	C	29	48.758	-12.338	71.165	1.00	21.63	C
ATOM	2719	C	LYS	C	29	49.976	-11.752	70.449	1.00	22.44	C
ATOM	2720	O	LYS	C	29	49.942	-11.521	69.242	1.00	24.06	O
ATOM	2721	CB	LYS	C	29	49.039	-13.827	71.405	1.00	22.39	C
ATOM	2722	CG	LYS	C	29	48.112	-14.554	72.354	1.00	22.12	C
ATOM	2723	CD	LYS	C	29	48.477	-16.031	72.387	1.00	21.48	C
ATOM	2724	CE	LYS	C	29	47.609	-16.835	73.353	1.00	21.29	C
ATOM	2725	NZ	LYS	C	29	47.777	-18.307	73.142	1.00	20.24	N
ATOM	2726	N	ASN	C	30	51.060	-11.541	71.184	1.00	23.38	N
ATOM	2727	CA	ASN	C	30	52.287	-11.026	70.584	1.00	25.47	C
ATOM	2728	C	ASN	C	30	53.269	-12.185	70.432	1.00	26.26	C
ATOM	2729	O	ASN	C	30	52.995	-13.297	70.889	1.00	25.69	O
ATOM	2730	CB	ASN	C	30	52.890	-9.893	71.419	1.00	27.31	C
ATOM	2731	CG	ASN	C	30	53.683	-10.385	72.611	1.00	30.17	C



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FIG. 53-47	ATOM 2733 ND2 ASN C 30	54.669 -9.604 73.011 1.00 35.07	N
	ATOM 2734 N SER C 31	54.432 -11.922 69.846 1.00 27.26	N
	ATOM 2735 CA SER C 31	55.423 -12.973 69.614 1.00 27.23	C
	ATOM 2736 C SER C 31	55.890 -13.745 70.852 1.00 27.63	C
	ATOM 2737 O SER C 31	56.648 -14.712 70.731 1.00 28.49	O
	ATOM 2738 CB SER C 31	56.625 -12.409 68.846 1.00 24.59	C
	ATOM 2739 OG SER C 31	57.292 -11.412 69.589 1.00 22.89	O
	ATOM 2740 N ASN C 32	55.424 -13.337 72.030 1.00 27.00	N
	ATOM 2741 CA ASN C 32	55.819 -13.990 73.282 1.00 25.25	C
	ATOM 2742 C ASN C 32	54.674 -14.735 73.959 1.00 24.89	C
	ATOM 2743 O ASN C 32	54.829 -15.233 75.074 1.00 25.83	O
	ATOM 2744 CB ASN C 32	56.402 -12.962 74.252 1.00 22.99	C
	ATOM 2745 CG ASN C 32	57.671 -12.330 73.730 1.00 23.34	C
	ATOM 2746 OD1 ASN C 32	58.726 -12.965 73.704 1.00 22.47	O
	ATOM 2747 ND2 ASN C 32	57.577 -11.078 73.293 1.00 23.40	N
	ATOM 2748 N GLN C 33	53.528 -14.806 73.285 1.00 23.19	N
	ATOM 2749 CA GLN C 33	52.346 -15.478 73.815 1.00 21.72	C
	ATOM 2750 C GLN C 33	51.613 -14.691 74.898 1.00 21.12	C
	ATOM 2751 O GLN C 33	50.781 -15.247 75.623 1.00 21.09	O
	ATOM 2752 CB GLN C 33	52.696 -16.888 74.306 1.00 21.85	C
	ATOM 2753 CG GLN C 33	52.808 -17.915 73.190 1.00 20.01	C
	ATOM 2754 CD GLN C 33	51.465 -18.245 72.588 1.00 18.26	C
	ATOM 2755 OE1 GLN C 33	50.641 -18.909 73.222 1.00 15.86	O
	ATOM 2756 NE2 GLN C 33	51.213 -17.746 71.379 1.00 17.44	N
	ATOM 2757 N ILE C 34	51.904 -13.397 74.991 1.00 20.10	N
	ATOM 2758 CA ILE C 34	51.249 -12.535 75.973 1.00 20.03	C
	ATOM 2759 C ILE C 34	49.875 -12.247 75.382 1.00 19.20	C
	ATOM 2760 O ILE C 34	49.766 -11.961 74.183 1.00 18.67	O
	ATOM 2761 CB ILE C 34	51.991 -11.169 76.140 1.00 21.24	C
	ATOM 2762 CG1 ILE C 34	53.457 -11.390 76.543 1.00 21.42	C
	ATOM 2763 CG2 ILE C 34	51.267 -10.287 77.159 1.00 18.98	C
	ATOM 2764 CD1 ILE C 34	53.647 -12.089 77.878 1.00 22.15	C
	ATOM 2765 N LYS C 35	48.832 -12.372 76.197 1.00 17.71	N
	ATOM 2766 CA LYS C 35	47.477 -12.111 75.724 1.00 16.90	C
	ATOM 2767 C LYS C 35	47.226 -10.606 75.642 1.00 17.56	C
	ATOM 2768 O LYS C 35	47.357 -9.880 76.635 1.00 16.09	O
	ATOM 2769 CB LYS C 35	46.437 -12.794 76.624 1.00 16.19	C
	ATOM 2770 CG LYS C 35	46.269 -14.292 76.376 1.00 15.00	C
	ATOM 2771 CD LYS C 35	46.569 -15.128 77.629 1.00 15.34	C
	ATOM 2772 CE LYS C 35	45.354 -15.350 78.508 1.00 12.17	C
	ATOM 2773 NZ LYS C 35	44.915 -14.132 79.227 1.00 16.76	N
	ATOM 2774 N ILE C 36	46.943 -10.139 74.432 1.00 17.78	N
	ATOM 2775 CA ILE C 36	46.669 -8.732 74.185 1.00 17.67	C
	ATOM 2776 C ILE C 36	45.164 -8.505 74.348 1.00 17.41	C
	ATOM 2777 O ILE C 36	44.725 -7.804 75.263 1.00 18.21	O
	ATOM 2778 CB ILE C 36	47.058 -8.318 72.729 1.00 17.98	C
	ATOM 2779 CG1 ILE C 36	48.523 -8.684 72.418 1.00 18.20	C
	ATOM 2780 CG2 ILE C 36	46.753 -6.837 72.495 1.00 14.26	C
	ATOM 2781 CD1 ILE C 36	49.593 -7.848 73.124 1.00 12.26	C
	ATOM 2782 N LEU C 37	44.381 -9.155 73.493 1.00 16.29	N
	ATOM 2783 CA LEU C 37	42.934 -8.997 73.499 1.00 16.37	C
	ATOM 2784 C LEU C 37	42.267 -10.310 73.110 1.00 16.74	C
	ATOM 2785 O LEU C 37	42.914 -11.212 72.584 1.00 19.68	O
	ATOM 2786 CB LEU C 37	42.552 -7.905 72.486 1.00 16.03	C
	ATOM 2787 CG LEU C 37	41.095 -7.454 72.339 1.00 15.19	C
	ATOM 2788 CD1 LEU C 37	40.926 -6.062 72.906 1.00 14.65	C
	ATOM 2789 CD2 LEU C 37	40.692 -7.490 70.864 1.00 17.32	C
	ATOM 2790 N GLY C 38	40.973 -10.416 73.375 1.00 14.89	N
	ATOM 2791 CA GLY C 38	40.232 -11.611 73.034 1.00 12.10	C
	ATOM 2792 C GLY C 38	38.857 -11.427 73.608 1.00 11.95	C
	ATOM 2793 O GLY C 38	38.597 -10.393 74.205 1.00 14.37	O
	ATOM 2794 N ASN C 39	37.973 -12.401 73.437 1.00 13.54	N
	ATOM 2795 CA ASN C 39	36.624 -12.295 73.984 1.00 14.16	C
	ATOM 2796 C ASN C 39	36.331 -13.486 74.885 1.00 14.77	C
	ATOM 2797 O ASN C 39	37.193 -14.350 75.090 1.00 15.40	O
	ATOM 2798 CB ASN C 39	35.567 -12.201 72.873 1.00 13.29	C
	ATOM 2799 CG ASN C 39	35.490 -13.460 72.013 1.00 15.65	C
	ATOM 2800 OD1 ASN C 39	35.976 -14.530 72.397 1.00 15.77	O
	ATOM 2801 ND2 ASN C 39	34.887 -13.333 70.833 1.00 12.54	N
	ATOM 2802 N GLN C 40	35.120 -13.488 75.450 1.00 13.54	N



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FIG. 53-48	ATOM 2804	C GLN C 40	33.139	-14.505	76.219	1.00	10.47	C
	ATOM 2805	O GLN C 40	32.444	-13.954	77.083	1.00	8.94	O
	ATOM 2806	CB GLN C 40	35.072	-14.327	77.793	1.00	10.26	C
	ATOM 2807	CG GLN C 40	36.433	-14.944	78.150	1.00	11.63	C
	ATOM 2808	CD GLN C 40	36.516	-16.464	77.940	1.00	11.02	C
	ATOM 2809	OE1 GLN C 40	37.565	-16.986	77.571	1.00	12.21	O
	ATOM 2810	NE2 GLN C 40	35.424	-17.173	78.204	1.00	7.03	N
	ATOM 2811	N GLY C 41	32.643	-15.095	75.136	1.00	10.34	N
	ATOM 2812	CA GLY C 41	31.218	-15.087	74.875	1.00	9.17	C
	ATOM 2813	C GLY C 41	30.964	-13.757	74.191	1.00	8.46	C
	ATOM 2814	O GLY C 41	31.518	-13.500	73.129	1.00	9.97	O
	ATOM 2815	N SER C 42	30.235	-12.872	74.855	1.00	7.34	N
	ATOM 2816	CA SER C 42	29.917	-11.560	74.310	1.00	5.83	C
	ATOM 2817	C SER C 42	30.754	-10.420	74.904	1.00	4.58	C
	ATOM 2818	O SER C 42	30.664	-9.262	74.467	1.00	2.00	O
	ATOM 2819	CB SER C 42	28.436	-11.281	74.535	1.00	7.62	C
	ATOM 2820	OG SER C 42	27.652	-12.282	73.918	1.00	7.72	O
	ATOM 2821	N PHE C 43	31.574	-10.756	75.894	1.00	4.84	N
	ATOM 2822	CA PHE C 43	32.412	-9.780	76.584	1.00	4.77	C
	ATOM 2823	C PHE C 43	33.851	-9.771	76.104	1.00	6.41	C
	ATOM 2824	O PHE C 43	34.401	-10.802	75.740	1.00	8.31	O
	ATOM 2825	CB PHE C 43	32.394	-10.062	78.085	1.00	3.80	C
	ATOM 2826	CG PHE C 43	31.019	-10.087	78.668	1.00	2.00	C
	ATOM 2827	CD1 PHE C 43	30.267	-8.927	78.734	1.00	2.00	C
	ATOM 2828	CD2 PHE C 43	30.467	-11.276	79.118	1.00	2.00	C
	ATOM 2829	CE1 PHE C 43	28.986	-8.945	79.232	1.00	2.13	C
	ATOM 2830	CE2 PHE C 43	29.174	-11.313	79.625	1.00	2.00	C
	ATOM 2831	CZ PHE C 43	28.429	-10.145	79.682	1.00	4.36	C
	ATOM 2832	N LEU C 44	34.468	-8.598	76.133	1.00	8.65	N
	ATOM 2833	CA LEU C 44	35.851	-8.448	75.712	1.00	10.75	C
	ATOM 2834	C LEU C 44	36.755	-8.770	76.898	1.00	10.90	C
	ATOM 2835	O LEU C 44	36.357	-8.616	78.042	1.00	11.48	O
	ATOM 2836	CB LEU C 44	36.105	-7.006	75.268	1.00	12.86	C
	ATOM 2837	CG LEU C 44	37.428	-6.748	74.547	1.00	14.62	C
	ATOM 2838	CD1 LEU C 44	37.262	-7.166	73.088	1.00	15.13	C
	ATOM 2839	CD2 LEU C 44	37.837	-5.277	74.664	1.00	13.01	C
	ATOM 2840	N THR C 45	37.973	-9.207	76.618	1.00	11.50	N
	ATOM 2841	CA THR C 45	38.928	-9.525	77.659	1.00	14.24	C
	ATOM 2842	C THR C 45	40.278	-9.018	77.191	1.00	16.99	C
	ATOM 2843	O THR C 45	40.656	-9.203	76.017	1.00	16.97	O
	ATOM 2844	CB THR C 45	39.036	-11.062	77.942	1.00	15.05	C
	ATOM 2845	OG1 THR C 45	39.389	-11.768	76.743	1.00	15.68	O
	ATOM 2846	CG2 THR C 45	37.724	-11.612	78.507	1.00	14.28	C
	ATOM 2847	N LYS C 46	40.980	-8.336	78.091	1.00	17.91	N
	ATOM 2848	CA LYS C 46	42.301	-7.808	77.788	1.00	17.33	C
	ATOM 2849	C LYS C 46	43.265	-8.506	78.714	1.00	17.01	C
	ATOM 2850	O LYS C 46	42.937	-8.764	79.875	1.00	18.56	O
	ATOM 2851	CB LYS C 46	42.372	-6.296	78.018	1.00	18.52	C
	ATOM 2852	CG LYS C 46	41.455	-5.474	77.133	1.00	18.34	C
	ATOM 2853	CD LYS C 46	41.807	-4.003	77.226	1.00	17.51	C
	ATOM 2854	CE LYS C 46	40.899	-3.181	76.336	1.00	19.67	C
	ATOM 2855	NZ LYS C 46	41.328	-1.760	76.203	1.00	18.93	N
	ATOM 2856	N GLY C 47	44.426	-8.858	78.184	1.00	16.02	N
	ATOM 2857	CA GLY C 47	45.426	-9.524	78.985	1.00	16.47	C
	ATOM 2858	C GLY C 47	46.391	-8.515	79.565	1.00	16.67	C
	ATOM 2859	O GLY C 47	46.124	-7.308	79.534	1.00	16.82	O
	ATOM 2860	N PROC 48	47.519	-8.981	80.125	1.00	16.94	N
	ATOM 2861	CA PROC 48	48.571	-8.155	80.732	1.00	16.26	C
	ATOM 2862	C PROC 48	49.466	-7.404	79.726	1.00	14.98	C
	ATOM 2863	O PROC 48	50.529	-6.903	80.094	1.00	15.58	O
	ATOM 2864	CB PROC 48	49.398	-9.191	81.509	1.00	14.81	C
	ATOM 2865	CG PROC 48	48.439	-10.289	81.772	1.00	14.85	C
	ATOM 2866	CD PROC 48	47.736	-10.400	80.455	1.00	15.47	C
	ATOM 2867	N SER C 49	49.050	-7.304	78.472	1.00	14.68	N
	ATOM 2868	CA SER C 49	49.878	-6.634	77.473	1.00	16.42	C
	ATOM 2869	C SER C 49	50.152	-5.176	77.805	1.00	17.17	C
	ATOM 2870	O SER C 49	49.384	-4.538	78.532	1.00	17.47	O
	ATOM 2871	CB SER C 49	49.221	-6.685	76.102	1.00	17.09	C
	ATOM 2872	OG SER C 49	48.311	-5.609	75.922	1.00	16.81	O
	ATOM 2873	N SER C 50	51.288	-4.633	77.306	1.00	18.51	N

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FIG. 53-49	ATOM 2875 C LYSC 50	50.643	-2.354	76.543	1.00	18.94	C
	ATOM 2876 O LYSC 50	50.795	-1.138	76.500	1.00	20.82	O
	ATOM 2877 CB LYSC 50	53.026	-2.991	77.078	1.00	21.26	C
	ATOM 2878 CG LYSC 50	53.540	-1.632	77.536	1.00	24.37	C
	ATOM 2879 CD LYSC 50	55.018	-1.463	77.232	1.00	27.45	C
	ATOM 2880 CE LYSC 50	55.500	-0.048	77.536	1.00	28.49	C
	ATOM 2881 NZ LYSC 50	56.905	0.162	77.095	1.00	25.44	N
	ATOM 2882 N LEUC 51	49.707	-2.986	75.837	1.00	19.14	N
	ATOM 2883 CA LEUC 51	48.735	-2.298	74.985	1.00	16.80	C
	ATOM 2884 C LEUC 51	47.399	-2.255	75.700	1.00	18.11	C
	ATOM 2885 O LEUC 51	46.454	-1.654	75.203	1.00	18.22	O
	ATOM 2886 CB LEUC 51	48.516	-3.065	73.676	1.00	12.49	C
	ATOM 2887 CG LEUC 51	49.483	-2.941	72.498	1.00	11.96	C
	ATOM 2888 CD1 LEUC 51	50.928	-3.201	72.901	1.00	9.37	C
	ATOM 2889 CD2 LEUC 51	49.034	-3.900	71.410	1.00	8.92	C
	ATOM 2890 N ASNC 52	47.318	-2.910	76.856	1.00	19.44	N
	ATOM 2891 CA ASNC 52	46.075	-3.000	77.623	1.00	21.42	C
	ATOM 2892 C ASNC 52	45.154	-1.793	77.526	1.00	21.58	C
	ATOM 2893 O ASNC 52	43.969	-1.910	77.186	1.00	21.08	O
	ATOM 2894 CB ASNC 52	46.374	-3.286	79.092	1.00	22.65	C
	ATOM 2895 CG ASNC 52	45.115	-3.524	79.897	1.00	25.24	C
	ATOM 2896 OD1 ASNC 52	44.399	-2.586	80.245	1.00	26.00	O
	ATOM 2897 ND2 ASNC 52	44.819	-4.787	80.169	1.00	27.41	N
	ATOM 2898 N ASPC 53	45.724	-0.635	77.821	1.00	22.99	N
	ATOM 2899 CA ASPC 53	45.017	0.641	77.810	1.00	22.76	C
	ATOM 2900 C ASPC 53	44.612	1.142	76.424	1.00	20.28	C
	ATOM 2901 O ASPC 53	43.583	1.808	76.287	1.00	20.58	O
	ATOM 2902 CB ASPC 53	45.883	1.688	78.510	1.00	27.19	C
	ATOM 2903 CG ASPC 53	47.369	1.438	78.304	1.00	32.20	C
	ATOM 2904 OD1 ASPC 53	47.834	1.474	77.140	1.00	34.77	O
	ATOM 2905 OD2 ASPC 53	48.063	1.153	79.304	1.00	33.85	O
	ATOM 2906 N ARG C 54	45.387	0.776	75.404	1.00	16.44	N
	ATOM 2907 CA ARG C 54	45.138	1.214	74.035	1.00	14.46	C
	ATOM 2908 C ARG C 54	44.498	0.223	73.052	1.00	15.26	C
	ATOM 2909 O ARG C 54	43.934	0.631	72.024	1.00	14.48	O
	ATOM 2910 CB ARG C 54	46.438	1.769	73.453	1.00	13.85	C
	ATOM 2911 CG ARG C 54	46.969	2.981	74.207	1.00	10.39	C
	ATOM 2912 CD ARG C 54	48.348	3.384	73.736	1.00	9.86	C
	ATOM 2913 NE ARG C 54	49.387	2.400	74.043	1.00	10.92	N
	ATOM 2914 CZ ARG C 54	49.902	1.546	73.159	1.00	11.74	C
	ATOM 2915 NH1 ARG C 54	49.465	1.539	71.903	1.00	10.30	N
	ATOM 2916 NH2 ARG C 54	50.884	0.731	73.521	1.00	11.51	N
	ATOM 2917 N ALA C 55	44.571	-1.066	73.362	1.00	15.91	N
	ATOM 2918 CA ALA C 55	44.012	-2.105	72.505	1.00	15.65	C
	ATOM 2919 C ALA C 55	42.538	-2.289	72.806	1.00	16.53	C
	ATOM 2920 O ALA C 55	42.146	-2.312	73.971	1.00	16.52	O
	ATOM 2921 CB ALA C 55	44.743	-3.414	72.735	1.00	16.20	C
	ATOM 2922 N ASP C 56	41.731	-2.424	71.759	1.00	16.49	N
	ATOM 2923 CA ASP C 56	40.289	-2.635	71.893	1.00	15.07	C
	ATOM 2924 C ASP C 56	39.804	-3.354	70.648	1.00	13.98	C
	ATOM 2925 O ASP C 56	40.599	-3.615	69.741	1.00	13.65	O
	ATOM 2926 CB ASP C 56	39.550	-1.316	72.086	1.00	15.99	C
	ATOM 2927 CG ASP C 56	38.751	-1.297	73.365	1.00	19.33	C
	ATOM 2928 OD1 ASP C 56	37.587	-1.749	73.338	1.00	18.87	O
	ATOM 2929 OD2 ASP C 56	39.301	-0.865	74.408	1.00	22.07	O
	ATOM 2930 N SER C 57	38.512	-3.642	70.568	1.00	13.07	N
	ATOM 2931 CA SER C 57	37.991	-4.388	69.421	1.00	12.85	C
	ATOM 2932 C SER C 57	36.819	-3.677	68.735	1.00	12.16	C
	ATOM 2933 O SER C 57	36.633	-2.468	68.873	1.00	9.84	O
	ATOM 2934 CB SER C 57	37.558	-5.783	69.913	1.00	12.60	C
	ATOM 2935 OG SER C 57	37.440	-6.721	68.858	1.00	14.97	O
	ATOM 2936 N ARG C 58	36.075	-4.420	67.925	1.00	12.21	N
	ATOM 2937 CA ARG C 58	34.897	-3.870	67.286	1.00	12.94	C
	ATOM 2938 C ARG C 58	33.805	-4.937	67.358	1.00	12.65	C
	ATOM 2939 O ARG C 58	33.483	-5.602	66.386	1.00	12.66	O
	ATOM 2940 CB ARG C 58	35.180	-3.396	65.860	1.00	13.06	C
	ATOM 2941 CG ARG C 58	34.391	-2.125	65.519	1.00	15.59	C
	ATOM 2942 CD ARG C 58	34.999	-1.326	64.364	1.00	16.20	C
	ATOM 2943 NE ARG C 58	34.536	0.057	64.369	1.00	16.31	N
	ATOM 2944 CZ ARG C 58	34.975	0.983	65.220	1.00	19.59	C

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FIG. 53-50	ATOM 2946 NH2 ARG C 58	34.474	2.211	65.191	1.00	21.55	N
	ATOM 2947 N ARG C 59	33.238	-5.063	68.551	1.00	13.04	N
	ATOM 2948 CA ARG C 59	32.187	-6.030	68.879	1.00	13.46	C
	ATOM 2949 C ARG C 59	31.102	-6.069	67.820	1.00	13.81	C
	ATOM 2950 O ARG C 59	30.430	-7.077	67.640	1.00	12.88	O
	ATOM 2951 CB ARG C 59	31.559	-5.658	70.225	1.00	12.47	C
	ATOM 2952 CG ARG C 59	32.574	-5.123	71.230	1.00	16.63	C
	ATOM 2953 CD ARG C 59	31.925	-4.363	72.377	1.00	15.86	C
	ATOM 2954 NE ARG C 59	31.447	-5.274	73.399	1.00	14.58	N
	ATOM 2955 CZ ARG C 59	32.094	-5.521	74.530	1.00	15.29	C
	ATOM 2956 NH1 ARG C 59	33.242	-4.907	74.793	1.00	11.07	N
	ATOM 2957 NH2 ARG C 59	31.651	-6.473	75.336	1.00	16.27	N
	ATOM 2958 N SER C 60	30.955	-4.952	67.119	1.00	15.22	N
	ATOM 2959 CA SER C 60	29.957	-4.780	66.074	1.00	14.35	C
	ATOM 2960 C SER C 60	30.115	-5.787	64.956	1.00	14.12	C
	ATOM 2961 O SER C 60	29.126	-6.249	64.391	1.00	14.24	O
	ATOM 2962 CB SER C 60	30.079	-3.373	65.491	1.00	13.29	C
	ATOM 2963 OG SER C 60	30.297	-2.413	66.513	1.00	12.44	O
	ATOM 2964 N LEU C 61	31.365	-6.114	64.643	1.00	13.35	N
	ATOM 2965 CA LEU C 61	31.698	-7.036	63.562	1.00	12.58	C
	ATOM 2966 C LEU C 61	31.890	-8.488	63.994	1.00	12.89	C
	ATOM 2967 O LEU C 61	32.214	-9.344	63.171	1.00	11.27	O
	ATOM 2968 CB LEU C 61	32.970	-6.542	62.861	1.00	12.99	C
	ATOM 2969 CG LEU C 61	32.986	-5.102	62.316	1.00	12.37	C
	ATOM 2970 CD1 LEU C 61	34.367	-4.729	61.845	1.00	10.21	C
	ATOM 2971 CD2 LEU C 61	32.002	-4.958	61.179	1.00	13.32	C
	ATOM 2972 N TRP C 62	31.653	-8.782	65.267	1.00	15.00	N
	ATOM 2973 CA TRP C 62	31.844	-10.137	65.768	1.00	15.79	C
	ATOM 2974 C TRP C 62	30.877	-11.111	65.138	1.00	17.16	C
	ATOM 2975 O TRP C 62	31.280	-12.199	64.708	1.00	16.99	O
	ATOM 2976 CB TRP C 62	31.737	-10.182	67.289	1.00	14.89	C
	ATOM 2977 CG TRP C 62	32.910	-9.553	67.997	1.00	12.85	C
	ATOM 2978 CD1 TRP C 62	33.989	-8.952	67.423	1.00	10.02	C
	ATOM 2979 CD2 TRP C 62	33.113	-9.470	69.418	1.00	11.04	C
	ATOM 2980 NE1 TRP C 62	34.846	-8.498	68.392	1.00	9.91	N
	ATOM 2981 CE2 TRP C 62	34.331	-8.798	69.625	1.00	8.87	C
	ATOM 2982 CE3 TRP C 62	32.379	-9.899	70.531	1.00	10.38	C
	ATOM 2983 CZ2 TRP C 62	34.840	-8.541	70.902	1.00	9.83	C
	ATOM 2984 CZ3 TRP C 62	32.884	-9.648	71.801	1.00	11.71	C
	ATOM 2985 CH2 TRP C 62	34.104	-8.971	71.975	1.00	10.91	C
	ATOM 2986 N ASP C 63	29.619	-10.689	65.023	1.00	18.68	N
	ATOM 2987 CA ASP C 63	28.560	-11.504	64.424	1.00	19.37	C
	ATOM 2988 C ASP C 63	28.674	-11.662	62.905	1.00	19.18	C
	ATOM 2989 O ASP C 63	27.858	-12.339	62.270	1.00	18.52	O
	ATOM 2990 CB ASP C 63	27.200	-10.939	64.801	1.00	20.43	C
	ATOM 2991 CG ASP C 63	27.000	-10.882	66.293	1.00	22.49	C
	ATOM 2992 OD1 ASP C 63	27.551	-11.753	67.000	1.00	22.01	O
	ATOM 2993 OD2 ASP C 63	26.310	-9.950	66.760	1.00	23.27	O
	ATOM 2994 N GLN C 64	29.665	-10.993	62.324	1.00	20.21	N
	ATOM 2995 CA GLN C 64	29.946	-11.072	60.894	1.00	21.25	C
	ATOM 2996 C GLN C 64	31.237	-11.861	60.695	1.00	21.70	C
	ATOM 2997 O GLN C 64	31.689	-12.079	59.566	1.00	21.95	O
	ATOM 2998 CB GLN C 64	30.060	-9.680	60.282	1.00	22.27	C
	ATOM 2999 CG GLN C 64	28.713	-9.092	59.868	1.00	27.63	C
	ATOM 3000 CD GLN C 64	27.617	-9.343	60.897	1.00	31.22	C
	ATOM 3001 OE1 GLN C 64	27.598	-8.736	61.971	1.00	32.64	O
	ATOM 3002 NE2 GLN C 64	26.718	-10.265	60.585	1.00	34.04	N
	ATOM 3003 N GLY C 65	31.812	-12.304	61.813	1.00	21.06	N
	ATOM 3004 CA GLY C 65	33.024	-13.090	61.776	1.00	19.23	C
	ATOM 3005 C GLY C 65	34.316	-12.317	61.841	1.00	19.06	C
	ATOM 3006 O GLY C 65	35.374	-12.928	61.888	1.00	20.04	O
	ATOM 3007 N ASN C 66	34.260	-10.991	61.859	1.00	18.88	N
	ATOM 3008 CA ASN C 66	35.487	-10.211	61.918	1.00	19.26	C
	ATOM 3009 C ASN C 66	35.736	-9.585	63.298	1.00	18.39	C
	ATOM 3010 O ASN C 66	34.952	-8.759	63.775	1.00	17.22	O
	ATOM 3011 CB ASN C 66	35.504	-9.142	60.816	1.00	22.32	C
	ATOM 3012 CG ASN C 66	36.770	-8.278	60.848	1.00	25.70	C
	ATOM 3013 OD1 ASN C 66	37.901	-8.784	60.827	1.00	26.05	O
	ATOM 3014 ND2 ASN C 66	36.578	-6.968	60.900	1.00	26.51	N
	ATOM 3015 N DHE C 67	36.817	-9.006	61.930	1.00	17.78	N

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FIG. 53-51

ATOM 3017	C PHE C 67	38.629	-8.895	65.173	1.00	15.42	C
ATOM 3018	O PHE C 67	39.629	-9.578	65.392	1.00	14.55	O
ATOM 3019	CB PHE C 67	37.261	-10.635	66.284	1.00	15.35	C
ATOM 3020	CG PHE C 67	36.638	-11.919	65.821	1.00	14.85	C
ATOM 3021	CD1 PHE C 67	37.409	-12.884	65.171	1.00	15.03	C
ATOM 3022	CD2 PHE C 67	35.299	-12.180	66.063	1.00	14.06	C
ATOM 3023	CE1 PHE C 67	36.866	-14.085	64.773	1.00	13.69	C
ATOM 3024	CE2 PHE C 67	34.737	-13.386	65.668	1.00	15.16	C
ATOM 3025	CZ PHE C 67	35.527	-14.343	65.021	1.00	15.92	C
ATOM 3026	N PRO C 68	38.709	-7.580	64.908	1.00	14.57	N
ATOM 3027	CA PRO C 68	39.975	-6.859	64.797	1.00	12.80	C
ATOM 3028	C PRO C 68	40.599	-6.423	66.117	1.00	11.73	C
ATOM 3029	O PRO C 68	39.979	-6.528	67.182	1.00	10.66	O
ATOM 3030	CB PRO C 68	39.581	-5.649	63.959	1.00	11.75	C
ATOM 3031	CG PRO C 68	38.226	-5.342	64.481	1.00	10.44	C
ATOM 3032	CD PRO C 68	37.576	-6.702	64.552	1.00	12.41	C
ATOM 3033	N LEU C 69	41.823	-5.905	66.012	1.00	10.60	N
ATOM 3034	CA LEU C 69	42.595	-5.395	67.140	1.00	10.14	C
ATOM 3035	C LEU C 69	42.793	-3.921	66.813	1.00	12.09	C
ATOM 3036	O LEU C 69	43.527	-3.583	65.870	1.00	14.51	O
ATOM 3037	CB LEU C 69	43.977	-6.051	67.181	1.00	7.25	C
ATOM 3038	CG LEU C 69	44.752	-6.202	68.495	1.00	6.79	C
ATOM 3039	CD1 LEU C 69	46.237	-6.243	68.179	1.00	5.65	C
ATOM 3040	CD2 LEU C 69	44.449	-5.091	69.477	1.00	2.33	C
ATOM 3041	N ILE C 70	42.145	-3.038	67.558	1.00	11.69	N
ATOM 3042	CA ILE C 70	42.286	-1.613	67.293	1.00	11.41	C
ATOM 3043	C ILE C 70	43.276	-0.974	68.255	1.00	11.83	C
ATOM 3044	O ILE C 70	42.932	-0.657	69.399	1.00	13.17	O
ATOM 3045	CB ILE C 70	40.937	-0.893	67.367	1.00	10.01	C
ATOM 3046	CG1 ILE C 70	40.002	-1.450	66.297	1.00	5.60	C
ATOM 3047	CG2 ILE C 70	41.129	0.603	67.162	1.00	11.59	C
ATOM 3048	CD1 ILE C 70	38.668	-0.798	66.297	1.00	5.00	C
ATOM 3049	N ILE C 71	44.502	-0.778	67.784	1.00	11.80	N
ATOM 3050	CA ILE C 71	45.554	-0.186	68.606	1.00	11.31	C
ATOM 3051	C ILE C 71	45.654	1.335	68.491	1.00	12.62	C
ATOM 3052	O ILE C 71	46.256	1.864	67.552	1.00	12.80	O
ATOM 3053	CB ILE C 71	46.927	-0.782	68.265	1.00	8.18	C
ATOM 3054	CG1 ILE C 71	46.898	-2.302	68.407	1.00	3.27	C
ATOM 3055	CG2 ILE C 71	47.993	-0.178	69.173	1.00	7.17	C
ATOM 3056	CD1 ILE C 71	48.127	-2.966	67.867	1.00	3.36	C
ATOM 3057	N LYS C 72	45.067	2.046	69.447	1.00	13.66	N
ATOM 3058	CA LYS C 72	45.149	3.493	69.412	1.00	13.73	C
ATOM 3059	C LYS C 72	46.495	3.954	69.953	1.00	12.76	C
ATOM 3060	O LYS C 72	47.207	3.195	70.607	1.00	11.55	O
ATOM 3061	CB LYS C 72	43.982	4.141	70.152	1.00	15.88	C
ATOM 3062	CG LYS C 72	43.750	3.668	71.563	1.00	18.88	C
ATOM 3063	CD LYS C 72	42.410	4.193	72.055	1.00	20.34	C
ATOM 3064	CE LYS C 72	41.521	3.058	72.523	1.00	23.79	C
ATOM 3065	NZ LYS C 72	41.542	1.869	71.616	1.00	26.10	N
ATOM 3066	N ASN C 73	46.870	5.173	69.592	1.00	13.66	N
ATOM 3067	CA ASN C 73	48.131	5.774	70.005	1.00	15.48	C
ATOM 3068	C ASN C 73	49.329	4.844	69.869	1.00	14.73	C
ATOM 3069	O ASN C 73	49.939	4.445	70.860	1.00	14.86	O
ATOM 3070	CB ASN C 73	48.036	6.315	71.430	1.00	16.97	C
ATOM 3071	CG ASN C 73	49.323	6.973	71.893	1.00	20.51	C
ATOM 3072	OD1 ASN C 73	49.654	6.944	73.088	1.00	23.06	O
ATOM 3073	ND2 ASN C 73	50.065	7.561	70.955	1.00	19.37	N
ATOM 3074	N LEU C 74	49.643	4.469	68.635	1.00	15.11	N
ATOM 3075	CA LEU C 74	50.787	3.603	68.388	1.00	14.53	C
ATOM 3076	C LEU C 74	52.020	4.234	69.004	1.00	15.55	C
ATOM 3077	O LEU C 74	52.154	5.467	69.054	1.00	15.44	O
ATOM 3078	CB LEU C 74	51.042	3.419	66.888	1.00	15.89	C
ATOM 3079	CG LEU C 74	50.184	2.525	65.982	1.00	15.23	C
ATOM 3080	CD1 LEU C 74	49.899	1.231	66.696	1.00	16.69	C
ATOM 3081	CD2 LEU C 74	48.907	3.206	65.600	1.00	14.58	C
ATOM 3082	N LYS C 75	52.895	3.388	69.515	1.00	17.06	N
ATOM 3083	CA LYS C 75	54.141	3.837	70.105	1.00	19.14	C
ATOM 3084	C LYS C 75	55.172	3.037	69.351	1.00	21.30	C
ATOM 3085	O LYS C 75	54.886	1.939	68.899	1.00	22.05	O
ATOM 3086	CB LYS C 75	54.104	2.403	71.501	1.00	18.02	C

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FIG. 53-52

ATOM	3088	CD	LYS	C	75	53.251	3.834	73.890	1.00	16.94	C
ATOM	3089	CE	LYS	C	75	52.035	4.287	74.678	1.00	16.82	C
ATOM	3090	NZ	LYS	C	75	51.586	5.625	74.222	1.00	17.55	N
ATOM	3091	N	ILE	C	76	56.366	3.582	69.179	1.00	23.77	N
ATOM	3092	CA	ILE	C	76	57.397	2.858	68.454	1.00	25.15	C
ATOM	3093	C	ILE	C	76	57.621	1.490	69.093	1.00	25.32	C
ATOM	3094	O	ILE	C	76	57.976	0.527	68.415	1.00	24.60	O
ATOM	3095	CB	ILE	C	76	58.707	3.680	68.393	1.00	26.22	C
ATOM	3096	CG1	ILE	C	76	58.587	4.749	67.303	1.00	27.32	C
ATOM	3097	CG2	ILE	C	76	59.913	2.781	68.102	1.00	25.80	C
ATOM	3098	CD1	ILE	C	76	57.491	5.768	67.529	1.00	26.34	C
ATOM	3099	N	GLU	C	77	57.312	1.403	70.384	1.00	26.79	N
ATOM	3100	CA	GLU	C	77	57.470	0.177	71.167	1.00	27.63	C
ATOM	3101	C	GLU	C	77	56.359	-0.863	70.974	1.00	26.10	C
ATOM	3102	O	GLU	C	77	56.429	-1.959	71.516	1.00	25.20	O
ATOM	3103	CB	GLU	C	77	57.655	0.523	72.655	1.00	29.66	C
ATOM	3104	CG	GLU	C	77	56.645	1.522	73.224	1.00	33.53	C
ATOM	3105	CD	GLU	C	77	56.970	1.950	74.645	1.00	36.75	C
ATOM	3106	OE1	GLU	C	77	57.926	1.408	75.231	1.00	39.53	O
ATOM	3107	OE2	GLU	C	77	56.266	2.820	75.199	1.00	39.29	O
ATOM	3108	N	ASP	C	78	55.346	-0.514	70.192	1.00	25.10	N
ATOM	3109	CA	ASP	C	78	54.249	-1.425	69.893	1.00	23.24	C
ATOM	3110	C	ASP	C	78	54.646	-2.320	68.724	1.00	22.69	C
ATOM	3111	O	ASP	C	78	53.898	-3.220	68.345	1.00	23.77	O
ATOM	3112	CB	ASP	C	78	52.982	-0.659	69.503	1.00	22.41	C
ATOM	3113	CG	ASP	C	78	52.318	0.027	70.677	1.00	22.01	C
ATOM	3114	OD1	ASP	C	78	52.715	-0.188	71.843	1.00	21.08	O
ATOM	3115	OD2	ASP	C	78	51.373	0.797	70.428	1.00	21.00	O
ATOM	3116	N	SER	C	79	55.792	-2.038	68.113	1.00	21.33	N
ATOM	3117	CA	SER	C	79	56.263	-2.832	66.990	1.00	19.92	C
ATOM	3118	C	SER	C	79	56.511	-4.258	67.461	1.00	20.47	C
ATOM	3119	O	SER	C	79	57.421	-4.516	68.258	1.00	19.43	O
ATOM	3120	CB	SER	C	79	57.542	-2.234	66.408	1.00	19.60	C
ATOM	3121	OG	SER	C	79	57.325	-0.905	65.968	1.00	17.97	O
ATOM	3122	N	ASP	C	80	55.683	-5.175	66.972	1.00	20.66	N
ATOM	3123	CA	ASP	C	80	55.773	-6.582	67.333	1.00	21.15	C
ATOM	3124	C	ASP	C	80	55.052	-7.351	66.237	1.00	21.82	C
ATOM	3125	O	ASP	C	80	54.693	-6.772	65.204	1.00	21.49	O
ATOM	3126	CB	ASP	C	80	55.076	-6.815	68.681	1.00	21.40	C
ATOM	3127	CG	ASP	C	80	55.637	-8.016	69.450	1.00	21.01	C
ATOM	3128	OD1	ASP	C	80	56.278	-8.896	68.832	1.00	20.07	O
ATOM	3129	OD2	ASP	C	80	55.421	-8.081	70.685	1.00	18.09	O
ATOM	3130	N	THR	C	81	54.842	-8.645	66.459	1.00	22.92	N
ATOM	3131	CA	THR	C	81	54.162	-9.517	65.506	1.00	22.30	C
ATOM	3132	C	THR	C	81	52.903	-10.027	66.196	1.00	20.64	C
ATOM	3133	O	THR	C	81	52.963	-10.666	67.247	1.00	20.88	O
ATOM	3134	CB	THR	C	81	55.069	-10.684	65.103	1.00	23.98	C
ATOM	3135	OG1	THR	C	81	56.333	-10.165	64.664	1.00	28.26	O
ATOM	3136	CG2	THR	C	81	54.454	-11.474	63.972	1.00	24.03	C
ATOM	3137	N	TYR	C	82	51.757	-9.696	65.624	1.00	19.53	N
ATOM	3138	CA	TYR	C	82	50.485	-10.074	66.205	1.00	18.75	C
ATOM	3139	C	TYR	C	82	49.865	-11.301	65.570	1.00	18.24	C
ATOM	3140	O	TYR	C	82	49.860	-11.462	64.349	1.00	17.98	O
ATOM	3141	CB	TYR	C	82	49.538	-8.865	66.200	1.00	18.14	C
ATOM	3142	CG	TYR	C	82	50.093	-7.730	67.034	1.00	13.90	C
ATOM	3143	CD1	TYR	C	82	49.875	-7.691	68.402	1.00	12.30	C
ATOM	3144	CD2	TYR	C	82	50.951	-6.772	66.473	1.00	14.05	C
ATOM	3145	CE1	TYR	C	82	50.500	-6.746	69.203	1.00	14.07	C
ATOM	3146	CE2	TYR	C	82	51.588	-5.819	67.270	1.00	12.70	C
ATOM	3147	CZ	TYR	C	82	51.360	-5.816	68.640	1.00	13.93	C
ATOM	3148	OH	TYR	C	82	52.008	-4.928	69.472	1.00	13.27	O
ATOM	3149	N	ILE	C	83	49.373	-12.180	66.434	1.00	17.52	N
ATOM	3150	CA	ILE	C	83	48.770	-13.437	66.030	1.00	16.78	C
ATOM	3151	C	ILE	C	83	47.307	-13.513	66.455	1.00	17.28	C
ATOM	3152	O	ILE	C	83	46.974	-13.255	67.610	1.00	17.58	O
ATOM	3153	CB	ILE	C	83	49.540	-14.626	66.652	1.00	15.69	C
ATOM	3154	CG1	ILE	C	83	50.902	-14.800	65.970	1.00	15.70	C
ATOM	3155	CG2	ILE	C	83	48.730	-15.889	66.557	1.00	15.51	C
ATOM	3156	CD1	ILE	C	83	52.029	-13.997	66.604	1.00	11.73	C
ATOM	3157	N	CYS	C	84	46.441	-13.880	65.522	1.00	18.23	N

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FIG. 53-53

ATOM 3159	C	CYSC 84	44.640	-15.483	65.814	1.00	24.15	C
ATOM 3160	O	CYSC 84	44.618	-16.154	64.766	1.00	22.78	O
ATOM 3161	CB	CYSC 84	44.188	-13.250	64.777	1.00	21.83	C
ATOM 3162	SG	CYSC 84	42.428	-13.182	65.225	1.00	25.21	S
ATOM 3163	N	GLUC 85	44.392	-15.994	67.018	1.00	27.19	N
ATOM 3164	CA	GLUC 85	44.015	-17.386	67.208	1.00	29.12	C
ATOM 3165	C	GLUC 85	42.507	-17.549	67.265	1.00	30.85	C
ATOM 3166	O	GLUC 85	41.885	-17.391	68.319	1.00	29.71	O
ATOM 3167	CB	GLUC 85	44.665	-17.947	68.475	1.00	28.74	C
ATOM 3168	CG	GLUC 85	46.187	-17.957	68.433	1.00	31.76	C
ATOM 3169	CD	GLUC 85	46.835	-18.225	69.780	1.00	34.21	C
ATOM 3170	OE1	GLUC 85	46.225	-17.912	70.825	1.00	33.71	O
ATOM 3171	OE2	GLUC 85	47.977	-18.739	69.797	1.00	37.16	O
ATOM 3172	N	VAL C 86	41.913	-17.733	66.092	1.00	34.16	N
ATOM 3173	CA	VAL C 86	40.480	-17.974	65.992	1.00	37.67	C
ATOM 3174	C	VAL C 86	40.445	-19.485	66.212	1.00	40.96	C
ATOM 3175	O	VAL C 86	41.444	-20.044	66.684	1.00	44.87	O
ATOM 3176	CB	VAL C 86	39.958	-17.638	64.591	1.00	37.29	C
ATOM 3177	CG1	VAL C 86	38.469	-17.369	64.643	1.00	38.34	C
ATOM 3178	CG2	VAL C 86	40.679	-16.434	64.040	1.00	36.92	C
ATOM 3179	N	GLUC 87	39.352	-20.172	65.894	1.00	41.57	N
ATOM 3180	CA	GLUC 87	39.351	-21.620	66.098	1.00	41.58	C
ATOM 3181	C	GLUC 87	40.342	-22.283	65.141	1.00	40.88	C
ATOM 3182	O	GLUC 87	40.013	-22.639	64.015	1.00	39.29	O
ATOM 3183	CB	GLUC 87	37.940	-22.198	65.976	1.00	43.78	C
ATOM 3184	CG	GLUC 87	37.021	-21.792	67.137	1.00	44.89	C
ATOM 3185	CD	GLUC 87	37.578	-22.178	68.514	1.00	45.97	C
ATOM 3186	OE1	GLUC 87	37.589	-23.384	68.848	1.00	46.01	O
ATOM 3187	OE2	GLUC 87	37.994	-21.271	69.269	1.00	45.49	O
ATOM 3188	N	ASPC 88	41.589	-22.311	65.593	1.00	42.51	N
ATOM 3189	CA	ASPC 88	42.743	-22.865	64.891	1.00	45.29	C
ATOM 3190	C	ASPC 88	43.083	-22.359	63.484	1.00	45.77	C
ATOM 3191	O	ASPC 88	42.784	-23.007	62.477	1.00	47.06	O
ATOM 3192	CB	ASPC 88	42.730	-24.395	64.926	1.00	47.66	C
ATOM 3193	CG	ASPC 88	44.050	-24.998	64.468	1.00	50.96	C
ATOM 3194	OD1	ASPC 88	45.112	-24.378	64.707	1.00	52.73	O
ATOM 3195	OD2	ASPC 88	44.020	-26.091	63.868	1.00	54.34	O
ATOM 3196	N	GLNC 89	43.686	-21.173	63.441	1.00	44.42	N
ATOM 3197	CA	GLNC 89	44.153	-20.531	62.213	1.00	43.08	C
ATOM 3198	C	GLNC 89	44.946	-19.302	62.657	1.00	42.12	C
ATOM 3199	O	GLNC 89	44.412	-18.209	62.856	1.00	43.48	O
ATOM 3200	CB	GLNC 89	43.019	-20.187	61.225	1.00	43.22	C
ATOM 3201	CG	GLNC 89	42.043	-19.084	61.612	1.00	45.08	C
ATOM 3202	CD	GLNC 89	41.334	-18.501	60.397	1.00	45.85	C
ATOM 3203	OE1	GLNC 89	41.128	-19.189	59.398	1.00	48.18	O
ATOM 3204	NE2	GLNC 89	40.962	-17.236	60.474	1.00	46.49	N
ATOM 3205	N	LYSC 90	46.231	-19.533	62.887	1.00	39.71	N
ATOM 3206	CA	LYSC 90	47.156	-18.513	63.353	1.00	36.88	C
ATOM 3207	C	LYSC 90	47.452	-17.390	62.340	1.00	36.11	C
ATOM 3208	O	LYSC 90	48.566	-17.305	61.814	1.00	36.72	O
ATOM 3209	CB	LYSC 90	48.459	-19.207	63.771	1.00	35.10	C
ATOM 3210	CG	LYSC 90	49.071	-18.718	65.069	1.00	33.77	C
ATOM 3211	CD	LYSC 90	48.474	-19.386	66.306	1.00	30.81	C
ATOM 3212	CE	LYSC 90	48.957	-20.826	66.463	1.00	28.79	C
ATOM 3213	NZ	LYSC 90	48.637	-21.374	67.809	1.00	25.63	N
ATOM 3214	N	GLUC 91	46.466	-16.542	62.050	1.00	34.49	N
ATOM 3215	CA	GLUC 91	46.675	-15.426	61.121	1.00	33.21	C
ATOM 3216	C	GLUC 91	47.696	-14.502	61.797	1.00	32.27	C
ATOM 3217	O	GLUC 91	47.449	-13.992	62.888	1.00	31.93	O
ATOM 3218	CB	GLUC 91	45.376	-14.653	60.895	1.00	34.08	C
ATOM 3219	CG	GLUC 91	44.211	-15.444	60.320	1.00	34.71	C
ATOM 3220	CD	GLUC 91	42.866	-14.887	60.777	1.00	35.45	C
ATOM 3221	OE1	GLUC 91	42.403	-15.312	61.851	1.00	37.00	O
ATOM 3222	OE2	GLUC 91	42.279	-14.020	60.090	1.00	34.33	O
ATOM 3223	N	GLUC 92	48.831	-14.284	61.149	1.00	30.93	N
ATOM 3224	CA	GLUC 92	49.898	-13.460	61.715	1.00	29.07	C
ATOM 3225	C	GLUC 92	50.055	-12.093	61.028	1.00	27.44	C
ATOM 3226	O	GLUC 92	49.619	-11.905	59.883	1.00	26.84	O
ATOM 3227	CB	GLUC 92	51.203	-14.259	61.626	1.00	29.91	C
ATOM 3228	CG	GLUC 92	52.383	-13.725	62.416	1.00	31.60	C

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FIG. 53-54	ATOM 3230	OE1 GLU C 92	54.115	-14.880	61.230	1.00	34.93	O
	ATOM 3231	OE2 GLU C 92	54.013	-15.165	63.409	1.00	32.07	O
	ATOM 3232	N VAL C 93	50.683	-11.147	61.726	1.00	25.33	N
	ATOM 3233	CA VAL C 93	50.925	-9.806	61.189	1.00	23.43	C
	ATOM 3234	C VAL C 93	52.093	-9.083	61.875	1.00	22.86	C
	ATOM 3235	O VAL C 93	52.321	-9.234	63.070	1.00	22.87	O
	ATOM 3236	CB VAL C 93	49.651	-8.914	61.251	1.00	22.01	C
	ATOM 3237	CG1 VAL C 93	49.281	-8.588	62.678	1.00	21.69	C
	ATOM 3238	CG2 VAL C 93	49.857	-7.644	60.453	1.00	20.43	C
	ATOM 3239	N GLN C 94	52.859	-8.330	61.098	1.00	24.05	N
	ATOM 3240	CA GLN C 94	53.986	-7.581	61.626	1.00	24.23	C
	ATOM 3241	C GLN C 94	53.602	-6.110	61.602	1.00	24.03	C
	ATOM 3242	O GLN C 94	53.295	-5.554	60.543	1.00	23.15	O
	ATOM 3243	CB GLN C 94	55.219	-7.823	60.765	1.00	27.34	C
	ATOM 3244	CG GLN C 94	56.502	-7.267	61.340	1.00	29.54	C
	ATOM 3245	CD GLN C 94	57.719	-7.813	60.629	1.00	30.13	C
	ATOM 3246	OE1 GLN C 94	58.107	-7.317	59.575	1.00	29.70	O
	ATOM 3247	NE2 GLN C 94	58.316	-8.857	61.193	1.00	30.59	N
	ATOM 3248	N LEU C 95	53.579	-5.498	62.782	1.00	22.86	N
	ATOM 3249	CA LEU C 95	53.205	-4.097	62.922	1.00	19.68	C
	ATOM 3250	C LEU C 95	54.424	-3.258	63.276	1.00	17.31	C
	ATOM 3251	O LEU C 95	55.025	-3.449	64.337	1.00	18.01	O
	ATOM 3252	CB LEU C 95	52.114	-3.959	63.995	1.00	19.68	C
	ATOM 3253	CG LEU C 95	51.338	-2.647	64.196	1.00	19.09	C
	ATOM 3254	CD1 LEU C 95	51.960	-1.830	65.312	1.00	19.14	C
	ATOM 3255	CD2 LEU C 95	51.231	-1.856	62.887	1.00	18.25	C
	ATOM 3256	N LEU C 96	54.818	-2.385	62.351	1.00	15.00	N
	ATOM 3257	CA LEU C 96	55.958	-1.486	62.533	1.00	14.64	C
	ATOM 3258	C LEU C 96	55.464	-0.058	62.726	1.00	14.32	C
	ATOM 3259	O LEU C 96	54.757	0.462	61.870	1.00	13.77	O
	ATOM 3260	CB LEU C 96	56.872	-1.502	61.301	1.00	12.86	C
	ATOM 3261	CG LEU C 96	57.840	-2.651	61.021	1.00	11.86	C
	ATOM 3262	CD1 LEU C 96	58.845	-2.759	62.140	1.00	10.73	C
	ATOM 3263	CD2 LEU C 96	57.093	-3.957	60.830	1.00	13.07	C
	ATOM 3264	N VAL C 97	55.830	0.580	63.832	1.00	15.46	N
	ATOM 3265	CA VAL C 97	55.412	1.964	64.056	1.00	17.77	C
	ATOM 3266	C VAL C 97	56.549	2.929	63.755	1.00	19.55	C
	ATOM 3267	O VAL C 97	57.657	2.775	64.276	1.00	20.22	O
	ATOM 3268	CB VAL C 97	54.908	2.213	65.483	1.00	16.29	C
	ATOM 3269	CG1 VAL C 97	54.597	3.676	65.659	1.00	15.45	C
	ATOM 3270	CG2 VAL C 97	53.655	1.391	65.743	1.00	18.13	C
	ATOM 3271	N PHE C 98	56.262	3.934	62.931	1.00	20.93	N
	ATOM 3272	CA PHE C 98	57.276	4.909	62.548	1.00	21.36	C
	ATOM 3273	C PHE C 98	56.982	6.307	63.032	1.00	22.58	C
	ATOM 3274	O PHE C 98	55.821	6.713	63.147	1.00	22.72	O
	ATOM 3275	CB PHE C 98	57.435	4.942	61.029	1.00	19.80	C
	ATOM 3276	CG PHE C 98	58.015	3.688	60.455	1.00	15.93	C
	ATOM 3277	CD1 PHE C 98	59.359	3.385	60.640	1.00	12.64	C
	ATOM 3278	CD2 PHE C 98	57.217	2.814	59.730	1.00	13.16	C
	ATOM 3279	CE1 PHE C 98	59.898	2.228	60.110	1.00	15.16	C
	ATOM 3280	CE2 PHE C 98	57.745	1.657	59.198	1.00	13.93	C
	ATOM 3281	CZ PHE C 98	59.087	1.358	59.384	1.00	14.61	C
	ATOM 3282	N GLY C 99	58.058	7.044	63.285	1.00	23.57	N
	ATOM 3283	CA GLY C 99	57.958	8.421	63.733	1.00	23.82	C
	ATOM 3284	C GLY C 99	58.810	9.247	62.793	1.00	22.91	C
	ATOM 3285	O GLY C 99	59.772	8.736	62.208	1.00	23.10	O
	ATOM 3286	N LEU C 100	58.448	10.510	62.619	1.00	22.42	N
	ATOM 3287	CA LEU C 100	59.184	11.398	61.729	1.00	21.39	C
	ATOM 3288	C LEU C 100	59.049	12.812	62.271	1.00	22.04	C
	ATOM 3289	O LEU C 100	58.090	13.519	61.969	1.00	21.68	O
	ATOM 3290	CB LEU C 100	58.606	11.287	60.312	1.00	20.03	C
	ATOM 3291	CG LEU C 100	59.312	11.872	59.089	1.00	17.21	C
	ATOM 3292	CD1 LEU C 100	58.976	13.336	58.940	1.00	18.15	C
	ATOM 3293	CD2 LEU C 100	60.810	11.635	59.176	1.00	16.63	C
	ATOM 3294	N THR C 101	59.985	13.199	63.124	1.00	23.11	N
	ATOM 3295	CA THR C 101	59.951	14.528	63.717	1.00	24.58	C
	ATOM 3296	C THR C 101	60.973	15.503	63.142	1.00	25.44	C
	ATOM 3297	O THR C 101	62.166	15.189	63.036	1.00	24.67	O
	ATOM 3298	CB THR C 101	60.111	14.460	65.254	1.00	23.29	C
	ATOM 3299	CG1 THR C 101	61.240	13.654	65.504	1.00	21.98	C

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FIG. 53-55	ATOM 3301	N	ALA C 102	60.485	16.670	62.733	1.00	27.01	N
	ATOM 3302	CA	ALA C 102	61.345	17.719	62.199	1.00	29.09	C
	ATOM 3303	C	ALA C 102	62.055	18.372	63.388	1.00	30.36	C
	ATOM 3304	O	ALA C 102	61.405	18.913	64.289	1.00	29.10	O
	ATOM 3305	CB	ALA C 102	60.514	18.749	61.431	1.00	27.84	C
	ATOM 3306	N	ASN C 103	63.377	18.241	63.421	1.00	32.41	N
	ATOM 3307	CA	ASN C 103	64.196	18.803	64.492	1.00	34.64	C
	ATOM 3308	C	ASN C 103	64.144	20.316	64.424	1.00	37.19	C
	ATOM 3309	O	ASN C 103	64.032	21.000	65.446	1.00	37.42	O
	ATOM 3310	CB	ASN C 103	65.667	18.378	64.349	1.00	32.99	C
	ATOM 3311	CG	ASN C 103	65.842	16.893	64.091	1.00	31.59	C
	ATOM 3312	OD1	ASN C 103	64.895	16.187	63.752	1.00	30.54	O
	ATOM 3313	ND2	ASN C 103	67.074	16.419	64.211	1.00	30.79	N
	ATOM 3314	N	SER C 104	64.192	20.829	63.200	1.00	39.57	N
	ATOM 3315	CA	SER C 104	64.200	22.264	62.938	1.00	41.79	C
	ATOM 3316	C	SER C 104	62.930	23.056	63.245	1.00	42.49	C
	ATOM 3317	O	SER C 104	62.711	24.110	62.640	1.00	43.24	O
	ATOM 3318	CB	SER C 104	64.606	22.493	61.486	1.00	41.64	C
	ATOM 3319	OG	SER C 104	65.582	21.542	61.099	1.00	43.50	O
	ATOM 3320	N	ASP C 105	62.112	22.584	64.187	1.00	42.26	N
	ATOM 3321	CA	ASP C 105	60.879	23.291	64.534	1.00	42.59	C
	ATOM 3322	C	ASP C 105	60.088	23.535	63.233	1.00	41.49	C
	ATOM 3323	O	ASP C 105	59.841	22.597	62.463	1.00	40.81	O
	ATOM 3324	CB	ASP C 105	61.221	24.619	65.266	1.00	44.61	C
	ATOM 3325	CG	ASP C 105	59.983	25.449	65.632	1.00	45.96	C
	ATOM 3326	OD1	ASP C 105	59.109	24.940	66.360	1.00	47.35	O
	ATOM 3327	OD2	ASP C 105	59.883	26.612	65.171	1.00	44.21	O
	ATOM 3328	N	THR C 106	59.742	24.794	62.971	1.00	39.76	N
	ATOM 3329	CA	THR C 106	59.001	25.195	61.789	1.00	37.14	C
	ATOM 3330	C	THR C 106	59.419	26.626	61.483	1.00	35.28	C
	ATOM 3331	O	THR C 106	59.939	26.889	60.400	1.00	36.37	O
	ATOM 3332	CB	THR C 106	57.452	25.137	61.985	1.00	37.13	C
	ATOM 3333	OG1	THR C 106	57.028	26.127	62.939	1.00	40.63	O
	ATOM 3334	CG2	THR C 106	57.010	23.763	62.449	1.00	36.75	C
	ATOM 3335	N	HIS C 107	59.241	27.529	62.451	1.00	32.22	N
	ATOM 3336	CA	HIS C 107	59.589	28.946	62.281	1.00	28.91	C
	ATOM 3337	C	HIS C 107	61.092	29.188	62.167	1.00	25.62	C
	ATOM 3338	O	HIS C 107	61.747	29.544	63.147	1.00	25.53	O
	ATOM 3339	CB	HIS C 107	59.049	29.780	63.439	1.00	29.99	C
	ATOM 3340	CG	HIS C 107	57.633	30.230	63.266	1.00	33.11	C
	ATOM 3341	ND1	HIS C 107	56.552	29.421	63.556	1.00	34.87	N
	ATOM 3342	CD2	HIS C 107	57.117	31.431	62.911	1.00	33.23	C
	ATOM 3343	CE1	HIS C 107	55.435	30.108	63.394	1.00	34.92	C
	ATOM 3344	NE2	HIS C 107	55.749	31.331	63.001	1.00	34.15	N
	ATOM 3345	N	LEU C 108	61.631	29.011	60.968	1.00	22.10	N
	ATOM 3346	CA	LEU C 108	63.050	29.207	60.725	1.00	18.56	C
	ATOM 3347	C	LEU C 108	63.240	30.371	59.778	1.00	16.16	C
	ATOM 3348	O	LEU C 108	62.281	30.923	59.255	1.00	16.77	O
	ATOM 3349	CB	LEU C 108	63.664	27.953	60.092	1.00	17.86	C
	ATOM 3350	CG	LEU C 108	63.637	26.645	60.880	1.00	17.69	C
	ATOM 3351	CD1	LEU C 108	63.980	25.503	59.969	1.00	18.79	C
	ATOM 3352	CD2	LEU C 108	64.612	26.702	62.026	1.00	19.44	C
	ATOM 3353	N	LEU C 109	64.496	30.716	59.537	1.00	14.36	N
	ATOM 3354	CA	LEU C 109	64.860	31.807	58.641	1.00	13.06	C
	ATOM 3355	C	LEU C 109	65.400	31.265	57.309	1.00	13.45	C
	ATOM 3356	O	LEU C 109	65.966	30.165	57.247	1.00	14.08	O
	ATOM 3357	CB	LEU C 109	65.933	32.682	59.306	1.00	10.18	C
	ATOM 3358	CG	LEU C 109	65.532	33.727	60.358	1.00	8.93	C
	ATOM 3359	CD1	LEU C 109	64.219	33.398	61.045	1.00	7.76	C
	ATOM 3360	CD2	LEU C 109	66.656	33.883	61.362	1.00	7.47	C
	ATOM 3361	N	GLN C 110	65.217	32.029	56.238	1.00	13.10	N
	ATOM 3362	CA	GLN C 110	65.728	31.617	54.944	1.00	13.18	C
	ATOM 3363	C	GLN C 110	67.235	31.434	55.148	1.00	12.96	C
	ATOM 3364	O	GLN C 110	67.888	32.272	55.777	1.00	13.50	O
	ATOM 3365	CB	GLN C 110	65.456	32.695	53.897	1.00	13.63	C
	ATOM 3366	CG	GLN C 110	63.999	33.126	53.822	1.00	14.21	C
	ATOM 3367	CD	GLN C 110	63.728	34.044	52.649	1.00	14.20	C
	ATOM 3368	OE1	GLN C 110	64.558	34.173	51.746	1.00	17.32	O
	ATOM 3369	NE2	GLN C 110	62.563	34.671	52.642	1.00	14.14	N
	ATOM 3370	N	GLN C 111	67.781	30.331	54.650	1.00	11.64	N



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FIG. 53-56	ATOM 3372	C	GLY C 111	69.411	29.082	55.965	1.00	9.44	C
	ATOM 3373	O	GLY C 111	70.521	28.591	56.172	1.00	7.92	O
	ATOM 3374	N	GLN C 112	68.348	28.797	56.715	1.00	8.64	N
	ATOM 3375	CA	GLN C 112	68.431	27.854	57.821	1.00	9.62	C
	ATOM 3376	C	GLN C 112	68.185	26.398	57.429	1.00	10.09	C
	ATOM 3377	O	GLN C 112	67.370	26.101	56.548	1.00	8.32	O
	ATOM 3378	CB	GLN C 112	67.503	28.274	58.945	1.00	9.21	C
	ATOM 3379	CG	GLN C 112	68.252	28.942	60.053	1.00	9.18	C
	ATOM 3380	CD	GLN C 112	67.408	29.901	60.831	1.00	8.46	C
	ATOM 3381	OE1	GLN C 112	67.772	31.061	60.980	1.00	10.11	O
	ATOM 3382	NE2	GLN C 112	66.280	29.431	61.344	1.00	8.06	N
	ATOM 3383	N	SER C 113	68.890	25.497	58.106	1.00	9.99	N
	ATOM 3384	CA	SER C 113	68.793	24.072	57.832	1.00	9.32	C
	ATOM 3385	C	SER C 113	67.532	23.443	58.361	1.00	9.91	C
	ATOM 3386	O	SER C 113	66.925	23.938	59.300	1.00	10.90	O
	ATOM 3387	CB	SER C 113	69.971	23.345	58.448	1.00	7.24	C
	ATOM 3388	OG	SER C 113	71.197	24.002	58.179	1.00	10.17	O
	ATOM 3389	N	LEU C 114	67.148	22.337	57.747	1.00	10.93	N
	ATOM 3390	CA	LEU C 114	65.972	21.587	58.157	1.00	9.91	C
	ATOM 3391	C	LEU C 114	66.532	20.203	58.413	1.00	9.55	C
	ATOM 3392	O	LEU C 114	67.512	19.807	57.778	1.00	10.78	O
	ATOM 3393	CB	LEU C 114	64.943	21.557	57.030	1.00	9.40	C
	ATOM 3394	CG	LEU C 114	63.558	20.933	57.208	1.00	9.41	C
	ATOM 3395	CD1	LEU C 114	63.611	19.422	57.055	1.00	11.32	C
	ATOM 3396	CD2	LEU C 114	62.964	21.329	58.524	1.00	8.77	C
	ATOM 3397	N	THR C 115	65.981	19.506	59.394	1.00	10.23	N
	ATOM 3398	CA	THR C 115	66.428	18.157	59.710	1.00	11.34	C
	ATOM 3399	C	THR C 115	65.248	17.340	60.211	1.00	12.00	C
	ATOM 3400	O	THR C 115	64.516	17.773	61.094	1.00	12.84	O
	ATOM 3401	CB	THR C 115	67.560	18.162	60.760	1.00	11.32	C
	ATOM 3402	OG1	THR C 115	68.714	18.828	60.231	1.00	13.64	O
	ATOM 3403	CG2	THR C 115	67.957	16.758	61.126	1.00	12.70	C
	ATOM 3404	N	LEU C 116	65.021	16.203	59.568	1.00	14.83	N
	ATOM 3405	CA	LEU C 116	63.938	15.286	59.920	1.00	17.05	C
	ATOM 3406	C	LEU C 116	64.579	14.013	60.466	1.00	17.08	C
	ATOM 3407	O	LEU C 116	65.514	13.483	59.861	1.00	16.50	O
	ATOM 3408	CB	LEU C 116	63.105	14.951	58.676	1.00	19.24	C
	ATOM 3409	CG	LEU C 116	62.368	16.126	58.024	1.00	22.16	C
	ATOM 3410	CD1	LEU C 116	61.885	15.728	56.663	1.00	24.14	C
	ATOM 3411	CD2	LEU C 116	61.201	16.561	58.888	1.00	23.58	C
	ATOM 3412	N	THR C 117	64.111	13.559	61.626	1.00	17.08	N
	ATOM 3413	CA	THR C 117	64.644	12.357	62.248	1.00	17.55	C
	ATOM 3414	C	THR C 117	63.606	11.247	62.186	1.00	18.51	C
	ATOM 3415	O	THR C 117	62.416	11.463	62.444	1.00	18.03	O
	ATOM 3416	CB	THR C 117	65.050	12.606	63.720	1.00	18.69	C
	ATOM 3417	OG1	THR C 117	65.874	13.773	63.803	1.00	19.51	O
	ATOM 3418	CG2	THR C 117	65.837	11.417	64.269	1.00	18.84	C
	ATOM 3419	N	LEU C 118	64.068	10.065	61.800	1.00	20.36	N
	ATOM 3420	CA	LEU C 118	63.223	8.891	61.683	1.00	21.54	C
	ATOM 3421	C	LEU C 118	63.245	8.114	62.989	1.00	23.23	C
	ATOM 3422	O	LEU C 118	64.313	7.700	63.449	1.00	23.33	O
	ATOM 3423	CB	LEU C 118	63.751	7.998	60.561	1.00	21.86	C
	ATOM 3424	CG	LEU C 118	62.976	6.721	60.224	1.00	22.93	C
	ATOM 3425	CD1	LEU C 118	61.767	7.052	59.348	1.00	20.94	C
	ATOM 3426	CD2	LEU C 118	63.909	5.754	59.516	1.00	23.45	C
	ATOM 3427	N	GLU C 119	62.079	7.960	63.608	1.00	25.58	N
	ATOM 3428	CA	GLU C 119	61.961	7.198	64.849	1.00	28.53	C
	ATOM 3429	C	GLU C 119	61.478	5.813	64.409	1.00	30.40	C
	ATOM 3430	O	GLU C 119	60.285	5.595	64.163	1.00	30.34	O
	ATOM 3431	CB	GLU C 119	60.960	7.858	65.798	1.00	28.11	C
	ATOM 3432	CG	GLU C 119	61.094	7.425	67.252	1.00	29.88	C
	ATOM 3433	CD	GLU C 119	60.427	8.391	68.222	1.00	32.15	C
	ATOM 3434	OE1	GLU C 119	59.438	9.056	67.845	1.00	32.83	O
	ATOM 3435	OE2	GLU C 119	60.902	8.510	69.366	1.00	34.00	O
	ATOM 3436	N	SER C 120	62.431	4.906	64.231	1.00	31.45	N
	ATOM 3437	CA	SER C 120	62.137	3.556	63.775	1.00	31.95	C
	ATOM 3438	C	SER C 120	62.286	2.504	64.869	1.00	31.72	C
	ATOM 3439	O	SER C 120	63.079	2.677	65.806	1.00	31.27	O
	ATOM 3440	CB	SER C 120	63.055	3.207	62.595	1.00	33.02	C
	ATOM 3441	CG	SER C 120	64.438	2.278	62.064	1.00	35.08	C

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FIG. 53-57	ATOM 3443	CA PRO C 121	61.528	0.276	65.702	1.00	32.79	C
	ATOM 3444	C PRO C 121	62.739	-0.637	65.541	1.00	33.59	C
	ATOM 3445	O PRO C 121	63.454	-0.578	64.537	1.00	34.27	O
	ATOM 3446	CB PRO C 121	60.244	-0.463	65.344	1.00	32.32	C
	ATOM 3447	CG PRO C 121	60.123	-0.223	63.882	1.00	31.58	C
	ATOM 3448	CD PRO C 121	60.439	1.239	63.775	1.00	30.99	C
	ATOM 3449	N PRO C 122	63.020	-1.457	66.560	1.00	34.59	N
	ATOM 3450	CA PRO C 122	64.146	-2.391	66.541	1.00	36.28	C
	ATOM 3451	C PRO C 122	64.024	-3.473	65.463	1.00	36.86	C
	ATOM 3452	O PRO C 122	63.143	-4.330	65.532	1.00	37.23	O
	ATOM 3453	CB PRO C 122	64.098	-2.998	67.943	1.00	37.24	C
	ATOM 3454	CG PRO C 122	63.611	-1.862	68.772	1.00	36.95	C
	ATOM 3455	CD PRO C 122	62.465	-1.345	67.921	1.00	36.11	C
	ATOM 3456	N GLY C 123	64.902	-3.415	64.465	1.00	37.07	N
	ATOM 3457	CA GLY C 123	64.884	-4.406	63.405	1.00	38.07	C
	ATOM 3458	C GLY C 123	64.528	-3.924	62.010	1.00	38.76	C
	ATOM 3459	O GLY C 123	64.528	-4.725	61.071	1.00	38.36	O
	ATOM 3460	N SER C 124	64.244	-2.632	61.851	1.00	39.57	N
	ATOM 3461	CA SER C 124	63.878	-2.095	60.544	1.00	40.33	C
	ATOM 3462	C SER C 124	64.870	-1.078	59.995	1.00	41.01	C
	ATOM 3463	O SER C 124	65.420	-0.270	60.751	1.00	41.37	O
	ATOM 3464	CB SER C 124	62.487	-1.462	60.608	1.00	39.66	C
	ATOM 3465	OG SER C 124	62.434	-0.456	61.606	1.00	39.35	O
	ATOM 3466	N SER C 125	65.060	-1.111	58.677	1.00	40.58	N
	ATOM 3467	CA SER C 125	65.951	-0.195	57.965	1.00	40.60	C
	ATOM 3468	C SER C 125	65.177	0.236	56.718	1.00	39.94	C
	ATOM 3469	O SER C 125	65.263	-0.411	55.670	1.00	40.98	O
	ATOM 3470	CB SER C 125	67.242	-0.916	57.551	1.00	41.65	C
	ATOM 3471	OG SER C 125	67.889	-1.526	58.657	1.00	42.74	O
	ATOM 3472	N PRO C 126	64.378	1.312	56.824	1.00	39.20	N
	ATOM 3473	CA PRO C 126	63.585	1.805	55.697	1.00	38.71	C
	ATOM 3474	C PRO C 126	64.209	2.964	54.926	1.00	38.11	C
	ATOM 3475	O PRO C 126	65.289	3.439	55.270	1.00	37.95	O
	ATOM 3476	CB PRO C 126	62.304	2.243	56.389	1.00	38.90	C
	ATOM 3477	CG PRO C 126	62.837	2.909	57.622	1.00	38.15	C
	ATOM 3478	CD PRO C 126	63.986	2.000	58.071	1.00	39.42	C
	ATOM 3479	N SER C 127	63.521	3.401	53.875	1.00	37.81	N
	ATOM 3480	CA SER C 127	63.972	4.528	53.062	1.00	38.14	C
	ATOM 3481	C SER C 127	62.956	5.661	53.161	1.00	38.67	C
	ATOM 3482	O SER C 127	61.754	5.437	53.026	1.00	39.41	O
	ATOM 3483	CB SER C 127	64.170	4.114	51.602	1.00	37.77	C
	ATOM 3484	OG SER C 127	65.456	3.535	51.401	1.00	38.00	O
	ATOM 3485	N VAL C 128	63.453	6.873	53.384	1.00	38.92	N
	ATOM 3486	CA VAL C 128	62.616	8.061	53.543	1.00	38.70	C
	ATOM 3487	C VAL C 128	62.735	8.998	52.341	1.00	38.75	C
	ATOM 3488	O VAL C 128	63.798	9.103	51.717	1.00	38.09	O
	ATOM 3489	CB VAL C 128	63.011	8.858	54.814	1.00	38.43	C
	ATOM 3490	CG1 VAL C 128	61.945	9.881	55.148	1.00	37.66	C
	ATOM 3491	CG2 VAL C 128	63.243	7.921	55.995	1.00	38.66	C
	ATOM 3492	N GLN C 129	61.644	9.705	52.051	1.00	38.20	N
	ATOM 3493	CA GLN C 129	61.580	10.649	50.936	1.00	37.25	C
	ATOM 3494	C GLN C 129	60.685	11.814	51.334	1.00	35.80	C
	ATOM 3495	O GLN C 129	59.489	11.629	51.574	1.00	35.49	O
	ATOM 3496	CB GLN C 129	61.018	9.951	49.687	1.00	38.46	C
	ATOM 3497	CG GLN C 129	60.652	10.861	48.511	1.00	41.45	C
	ATOM 3498	CD GLN C 129	59.143	11.067	48.350	1.00	43.36	C
	ATOM 3499	OE1 GLN C 129	58.334	10.276	48.843	1.00	43.93	O
	ATOM 3500	NE2 GLN C 129	58.763	12.130	47.648	1.00	41.25	N
	ATOM 3501	N CYS C 130	61.270	13.000	51.456	1.00	34.06	N
	ATOM 3502	CA CYS C 130	60.501	14.183	51.817	1.00	32.97	C
	ATOM 3503	C CYS C 130	60.526	15.161	50.660	1.00	31.87	C
	ATOM 3504	O CYS C 130	61.581	15.415	50.081	1.00	31.95	O
	ATOM 3505	CB CYS C 130	61.075	14.859	53.063	1.00	34.29	C
	ATOM 3506	SG CYS C 130	60.956	13.916	54.615	1.00	34.97	S
	ATOM 3507	N ARG C 131	59.362	15.711	50.333	1.00	30.51	N
	ATOM 3508	CA ARG C 131	59.233	16.655	49.238	1.00	28.80	C
	ATOM 3509	C ARG C 131	58.691	17.965	49.800	1.00	27.51	C
	ATOM 3510	O ARG C 131	57.660	17.982	50.475	1.00	26.63	O
	ATOM 3511	CB ARG C 131	58.277	16.085	48.190	1.00	29.85	C
	ATOM 3512	CG ARG C 131	58.233	16.878	46.877	1.00	33.23	C

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FIG. 53-58	ATOM 3514	NE ARG C 131	58.861	16.759	44.505	1.00	38.86	N
	ATOM 3515	CZ ARG C 131	59.210	16.182	43.357	1.00	40.02	C
	ATOM 3516	NH1 ARG C 131	59.868	15.028	43.361	1.00	40.08	N
	ATOM 3517	NH2 ARG C 131	58.880	16.751	42.202	1.00	39.80	N
	ATOM 3518	N SER C 132	59.417	19.049	49.549	1.00	25.96	N
	ATOM 3519	CA SER C 132	59.045	20.383	50.013	1.00	24.47	C
	ATOM 3520	C SER C 132	57.892	20.928	49.185	1.00	23.51	C
	ATOM 3521	O SER C 132	57.597	20.409	48.105	1.00	24.24	O
	ATOM 3522	CB SER C 132	60.235	21.332	49.873	1.00	23.44	C
	ATOM 3523	OG SER C 132	60.485	21.586	48.506	1.00	20.32	O
	ATOM 3524	N PRO C 133	57.258	22.018	49.647	1.00	22.71	N
	ATOM 3525	CA PRO C 133	56.141	22.608	48.909	1.00	21.46	C
	ATOM 3526	C PRO C 133	56.516	22.930	47.464	1.00	21.15	C
	ATOM 3527	O PRO C 133	55.660	22.899	46.585	1.00	21.36	O
	ATOM 3528	CB PRO C 133	55.849	23.868	49.711	1.00	19.38	C
	ATOM 3529	CG PRO C 133	56.170	23.441	51.096	1.00	18.92	C
	ATOM 3530	CD PRO C 133	57.470	22.733	50.917	1.00	21.34	C
	ATOM 3531	N ARG C 134	57.797	23.222	47.224	1.00	21.78	N
	ATOM 3532	CA ARG C 134	58.285	23.541	45.878	1.00	21.34	C
	ATOM 3533	C ARG C 134	58.969	22.372	45.150	1.00	21.00	C
	ATOM 3534	O ARG C 134	59.787	22.569	44.251	1.00	21.10	O
	ATOM 3535	CB ARG C 134	59.183	24.788	45.893	1.00	20.36	C
	ATOM 3536	CG ARG C 134	60.260	24.810	46.968	1.00	21.80	C
	ATOM 3537	CD ARG C 134	61.635	24.362	46.458	1.00	24.10	C
	ATOM 3538	NE ARG C 134	62.653	24.468	47.507	1.00	24.28	N
	ATOM 3539	CZ ARG C 134	63.968	24.506	47.306	1.00	24.06	C
	ATOM 3540	NH1 ARG C 134	64.473	24.444	46.084	1.00	24.86	N
	ATOM 3541	NH2 ARG C 134	64.775	24.674	48.339	1.00	26.77	N
	ATOM 3542	N GLY C 135	58.621	21.150	45.537	1.00	20.48	N
	ATOM 3543	CA GLY C 135	59.185	19.978	44.892	1.00	17.34	C
	ATOM 3544	C GLY C 135	60.623	19.629	45.222	1.00	15.25	C
	ATOM 3545	O GLY C 135	61.174	18.715	44.616	1.00	15.64	O
	ATOM 3546	N LYS C 136	61.247	20.364	46.136	1.00	13.71	N
	ATOM 3547	CA LYS C 136	62.625	20.072	46.536	1.00	13.59	C
	ATOM 3548	C LYS C 136	62.572	18.805	47.398	1.00	13.78	C
	ATOM 3549	O LYS C 136	61.961	18.813	48.464	1.00	12.87	O
	ATOM 3550	CB LYS C 136	63.207	21.257	47.335	1.00	13.17	C
	ATOM 3551	CG LYS C 136	64.350	20.921	48.304	1.00	11.86	C
	ATOM 3552	CD LYS C 136	65.713	21.282	47.752	1.00	8.91	C
	ATOM 3553	CE LYS C 136	66.821	20.647	48.565	1.00	9.07	C
	ATOM 3554	NZ LYS C 136	66.698	19.152	48.557	1.00	12.43	N
	ATOM 3555	N ASN C 137	63.173	17.712	46.938	1.00	15.38	N
	ATOM 3556	CA ASN C 137	63.130	16.487	47.728	1.00	16.86	C
	ATOM 3557	C ASN C 137	64.450	16.008	48.325	1.00	16.82	C
	ATOM 3558	O ASN C 137	65.529	16.277	47.801	1.00	16.16	O
	ATOM 3559	CB ASN C 137	62.399	15.354	46.988	1.00	19.19	C
	ATOM 3560	CG ASN C 137	63.016	15.023	45.649	1.00	21.52	C
	ATOM 3561	OD1 ASN C 137	62.582	15.540	44.604	1.00	21.42	O
	ATOM 3562	ND2 ASN C 137	63.998	14.119	45.652	1.00	22.72	N
	ATOM 3563	N ILE C 138	64.341	15.381	49.488	1.00	17.42	N
	ATOM 3564	CA ILE C 138	65.479	14.854	50.227	1.00	17.65	C
	ATOM 3565	C ILE C 138	65.213	13.366	50.497	1.00	18.77	C
	ATOM 3566	O ILE C 138	64.070	12.968	50.772	1.00	17.83	O
	ATOM 3567	CB ILE C 138	65.695	15.651	51.540	1.00	16.36	C
	ATOM 3568	CG1 ILE C 138	64.376	15.799	52.308	1.00	16.75	C
	ATOM 3569	CG2 ILE C 138	66.221	17.040	51.213	1.00	15.86	C
	ATOM 3570	CD1 ILE C 138	64.500	16.523	53.648	1.00	15.58	C
	ATOM 3571	N GLN C 139	66.262	12.552	50.375	1.00	19.50	N
	ATOM 3572	CA GLN C 139	66.157	11.108	50.556	1.00	21.45	C
	ATOM 3573	C GLN C 139	67.162	10.595	51.571	1.00	21.93	C
	ATOM 3574	O GLN C 139	68.333	10.949	51.509	1.00	23.09	O
	ATOM 3575	CB GLN C 139	66.363	10.374	49.219	1.00	23.24	C
	ATOM 3576	CG GLN C 139	66.679	11.249	47.986	1.00	27.09	C
	ATOM 3577	CD GLN C 139	68.030	11.970	48.048	1.00	29.61	C
	ATOM 3578	OE1 GLN C 139	68.177	13.075	47.520	1.00	28.85	O
	ATOM 3579	NE2 GLN C 139	69.014	11.353	48.690	1.00	30.92	N
	ATOM 3580	N GLY C 140	66.712	9.743	52.484	1.00	22.40	N
	ATOM 3581	CA GLY C 140	67.603	9.202	53.499	1.00	24.32	C
	ATOM 3582	C GLY C 140	66.971	8.072	54.297	1.00	25.45	C
	ATOM 3583	O GLY C 140	65.848	7.663	54.003	1.00	25.77	O

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FIG. 53-59	ATOM 3585 CA GLY C 141	67.098	6.508	56.119	1.00	24.09	C
	ATOM 3586 C GLY C 141	67.280	6.660	57.613	1.00	24.16	C
	ATOM 3587 O GLY C 141	67.559	5.690	58.317	1.00	25.48	O
	ATOM 3588 N LYS C 142	67.118	7.882	58.097	1.00	23.81	N
	ATOM 3589 CA LYS C 142	67.259	8.190	59.512	1.00	23.83	C
	ATOM 3590 C LYS C 142	67.099	9.701	59.623	1.00	23.09	C
	ATOM 3591 O LYS C 142	66.019	10.199	59.942	1.00	22.51	O
	ATOM 3592 CB LYS C 142	68.634	7.752	60.044	1.00	24.56	C
	ATOM 3593 CG LYS C 142	68.791	7.800	61.572	1.00	27.42	C
	ATOM 3594 CD LYS C 142	68.575	6.433	62.239	1.00	25.14	C
	ATOM 3595 CE LYS C 142	67.124	5.972	62.149	1.00	27.04	C
	ATOM 3596 NZ LYS C 142	66.894	4.599	62.699	1.00	27.76	N
	ATOM 3597 N THR C 143	68.146	10.433	59.271	1.00	21.45	N
	ATOM 3598 CA THR C 143	68.074	11.874	59.348	1.00	20.52	C
	ATOM 3599 C THR C 143	68.160	12.497	57.965	1.00	20.63	C
	ATOM 3600 O THR C 143	69.124	12.279	57.233	1.00	20.70	O
	ATOM 3601 CB THR C 143	69.150	12.455	60.295	1.00	20.16	C
	ATOM 3602 OG1 THR C 143	68.901	13.850	60.504	1.00	22.12	O
	ATOM 3603 CG2 THR C 143	70.558	12.259	59.737	1.00	17.82	C
	ATOM 3604 N LEU C 144	67.093	13.170	57.565	1.00	20.19	N
	ATOM 3605 CA LEU C 144	67.083	13.839	56.280	1.00	19.88	C
	ATOM 3606 C LEU C 144	67.425	15.298	56.533	1.00	20.01	C
	ATOM 3607 O LEU C 144	67.055	15.877	57.565	1.00	18.86	O
	ATOM 3608 CB LEU C 144	65.725	13.721	55.587	1.00	19.27	C
	ATOM 3609 CG LEU C 144	65.468	12.475	54.744	1.00	17.79	C
	ATOM 3610 CD1 LEU C 144	65.432	11.262	55.631	1.00	17.30	C
	ATOM 3611 CD2 LEU C 144	64.148	12.627	54.018	1.00	17.18	C
	ATOM 3612 N SER C 145	68.153	15.891	55.602	1.00	19.94	N
	ATOM 3613 CA SER C 145	68.533	17.273	55.762	1.00	20.38	C
	ATOM 3614 C SER C 145	68.385	18.092	54.492	1.00	20.97	C
	ATOM 3615 O SER C 145	68.109	17.562	53.411	1.00	22.10	O
	ATOM 3616 CB SER C 145	69.972	17.351	56.259	1.00	18.81	C
	ATOM 3617 OG SER C 145	70.087	16.818	57.558	1.00	14.54	O
	ATOM 3618 N VAL C 146	68.515	19.400	54.677	1.00	19.20	N
	ATOM 3619 CA VAL C 146	68.462	20.405	53.628	1.00	17.60	C
	ATOM 3620 C VAL C 146	69.337	21.460	54.287	1.00	18.03	C
	ATOM 3621 O VAL C 146	68.974	21.994	55.345	1.00	18.89	O
	ATOM 3622 CB VAL C 146	67.055	21.002	53.461	1.00	16.34	C
	ATOM 3623 CG1 VAL C 146	67.002	21.849	52.211	1.00	16.62	C
	ATOM 3624 CG2 VAL C 146	65.996	19.913	53.420	1.00	16.04	C
	ATOM 3625 N SER C 147	70.531	21.681	53.743	1.00	17.43	N
	ATOM 3626 CA SER C 147	71.447	22.658	54.329	1.00	15.43	C
	ATOM 3627 C SER C 147	70.859	24.070	54.415	1.00	13.97	C
	ATOM 3628 O SER C 147	70.756	24.631	55.502	1.00	12.41	O
	ATOM 3629 CB SER C 147	72.792	22.655	53.587	1.00	16.46	C
	ATOM 3630 OG SER C 147	72.644	22.912	52.196	1.00	17.35	O
	ATOM 3631 N GLN C 148	70.466	24.630	53.276	1.00	13.00	N
	ATOM 3632 CA GLN C 148	69.890	25.969	53.232	1.00	11.88	C
	ATOM 3633 C GLN C 148	68.450	25.897	52.755	1.00	9.40	C
	ATOM 3634 O GLN C 148	68.160	25.281	51.745	1.00	10.44	O
	ATOM 3635 CB GLN C 148	70.704	26.893	52.309	1.00	12.05	C
	ATOM 3636 CG GLN C 148	70.103	28.301	52.175	1.00	17.81	C
	ATOM 3637 CD GLN C 148	70.838	29.218	51.190	1.00	19.20	C
	ATOM 3638 OE1 GLN C 148	71.948	29.672	51.464	1.00	22.13	O
	ATOM 3639 NE2 GLN C 148	70.191	29.540	50.071	1.00	15.41	N
	ATOM 3640 N LEU C 149	67.548	26.462	53.542	1.00	9.65	N
	ATOM 3641 CA LEU C 149	66.132	26.510	53.211	1.00	8.56	C
	ATOM 3642 C LEU C 149	65.949	27.755	52.372	1.00	10.00	C
	ATOM 3643 O LEU C 149	66.798	28.656	52.375	1.00	9.13	O
	ATOM 3644 CB LEU C 149	65.274	26.641	54.479	1.00	6.97	C
	ATOM 3645 CG LEU C 149	64.448	25.444	54.966	1.00	5.33	C
	ATOM 3646 CD1 LEU C 149	65.267	24.169	54.903	1.00	7.70	C
	ATOM 3647 CD2 LEU C 149	63.960	25.700	56.376	1.00	5.54	C
	ATOM 3648 N GLU C 150	64.811	27.823	51.702	1.00	10.94	N
	ATOM 3649 CA GLU C 150	64.480	28.941	50.850	1.00	12.11	C
	ATOM 3650 C GLU C 150	63.058	29.318	51.215	1.00	12.07	C
	ATOM 3651 O GLU C 150	62.311	28.498	51.738	1.00	11.71	O
	ATOM 3652 CB GLU C 150	64.583	28.533	49.374	1.00	14.71	C
	ATOM 3653 CG GLU C 150	66.006	28.167	48.918	1.00	18.45	C
	ATOM 3654 CD GLU C 150	66.051	29.372	48.877	1.00	21.02	C

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FIG. 53-60	ATOM 3656	OE2 GLU C 150	67.340	29.775	47.766	1.00	21.00	O
	ATOM 3657	N LEU C 151	62.694	30.569	50.972	1.00	11.69	N
	ATOM 3658	CA LEU C 151	61.365	31.052	51.293	1.00	11.57	C
	ATOM 3659	C LEU C 151	60.289	30.112	50.790	1.00	12.44	C
	ATOM 3660	O LEU C 151	59.308	29.851	51.494	1.00	13.93	O
	ATOM 3661	CB LEU C 151	61.158	32.447	50.709	1.00	12.37	C
	ATOM 3662	CG LEU C 151	59.797	33.113	50.883	1.00	13.90	C
	ATOM 3663	CD1 LEU C 151	59.406	33.231	52.352	1.00	13.05	C
	ATOM 3664	CD2 LEU C 151	59.879	34.479	50.249	1.00	16.05	C
	ATOM 3665	N GLN C 152	60.507	29.536	49.613	1.00	12.55	N
	ATOM 3666	CA GLN C 152	59.515	28.641	49.028	1.00	11.90	C
	ATOM 3667	C GLN C 152	59.396	27.259	49.666	1.00	12.70	C
	ATOM 3668	O GLN C 152	58.599	26.433	49.209	1.00	13.13	O
	ATOM 3669	CB GLN C 152	59.707	28.529	47.519	1.00	11.46	C
	ATOM 3670	CG GLN C 152	59.413	29.818	46.770	1.00	8.15	C
	ATOM 3671	CD GLN C 152	60.596	30.768	46.760	1.00	9.54	C
	ATOM 3672	OE1 GLN C 152	61.649	30.483	47.339	1.00	8.38	O
	ATOM 3673	NE2 GLN C 152	60.441	31.897	46.080	1.00	11.22	N
	ATOM 3674	N ASP C 153	60.175	27.014	50.719	1.00	12.72	N
	ATOM 3675	CA ASP C 153	60.119	25.749	51.439	1.00	11.31	C
	ATOM 3676	C ASP C 153	59.047	25.834	52.519	1.00	12.42	C
	ATOM 3677	O ASP C 153	58.768	24.854	53.191	1.00	13.71	O
	ATOM 3678	CB ASP C 153	61.462	25.409	52.096	1.00	9.61	C
	ATOM 3679	CG ASP C 153	62.505	24.929	51.103	1.00	9.74	C
	ATOM 3680	OD1 ASP C 153	62.285	23.937	50.394	1.00	9.94	O
	ATOM 3681	OD2 ASP C 153	63.587	25.527	51.039	1.00	12.49	O
	ATOM 3682	N SER C 154	58.438	27.001	52.693	1.00	14.62	N
	ATOM 3683	CA SER C 154	57.407	27.158	53.712	1.00	15.40	C
	ATOM 3684	C SER C 154	56.109	26.507	53.270	1.00	17.42	C
	ATOM 3685	O SER C 154	55.578	26.816	52.206	1.00	18.74	O
	ATOM 3686	CB SER C 154	57.183	28.639	54.034	1.00	14.80	C
	ATOM 3687	OG SER C 154	56.473	28.813	55.254	1.00	10.64	O
	ATOM 3688	N GLY C 155	55.599	25.612	54.105	1.00	18.91	N
	ATOM 3689	CA GLY C 155	54.367	24.920	53.794	1.00	19.59	C
	ATOM 3690	C GLY C 155	54.402	23.508	54.352	1.00	21.01	C
	ATOM 3691	O GLY C 155	55.160	23.211	55.279	1.00	19.93	O
	ATOM 3692	N THR C 156	53.612	22.621	53.758	1.00	21.99	N
	ATOM 3693	CA THR C 156	53.550	21.241	54.209	1.00	22.98	C
	ATOM 3694	C THR C 156	54.474	20.346	53.402	1.00	22.60	C
	ATOM 3695	O THR C 156	54.344	20.257	52.180	1.00	25.02	O
	ATOM 3696	CB THR C 156	52.125	20.678	54.086	1.00	24.04	C
	ATOM 3697	OG1 THR C 156	51.235	21.385	54.958	1.00	25.86	O
	ATOM 3698	CG2 THR C 156	52.111	19.219	54.432	1.00	25.42	C
	ATOM 3699	N TRP C 157	55.421	19.713	54.086	1.00	21.34	N
	ATOM 3700	CA TRP C 157	56.359	18.781	53.463	1.00	19.59	C
	ATOM 3701	C TRP C 157	55.717	17.395	53.513	1.00	20.25	C
	ATOM 3702	O TRP C 157	54.974	17.092	54.450	1.00	20.58	O
	ATOM 3703	CB TRP C 157	57.679	18.753	54.234	1.00	15.84	C
	ATOM 3704	CG TRP C 157	58.513	19.987	54.077	1.00	11.16	C
	ATOM 3705	CD1 TRP C 157	58.089	21.282	54.161	1.00	11.79	C
	ATOM 3706	CD2 TRP C 157	59.911	20.041	53.762	1.00	8.24	C
	ATOM 3707	NE1 TRP C 157	59.132	22.138	53.907	1.00	9.41	N
	ATOM 3708	CE2 TRP C 157	60.263	21.405	53.657	1.00	8.97	C
	ATOM 3709	CE3 TRP C 157	60.900	19.068	53.558	1.00	6.12	C
	ATOM 3710	CZ2 TRP C 157	61.564	21.826	53.353	1.00	9.57	C
	ATOM 3711	CZ3 TRP C 157	62.192	19.482	53.256	1.00	8.10	C
	ATOM 3712	CH2 TRP C 157	62.513	20.852	53.156	1.00	10.47	C
	ATOM 3713	N THR C 158	55.976	16.569	52.501	1.00	21.03	N
	ATOM 3714	CA THR C 158	55.418	15.218	52.449	1.00	20.80	C
	ATOM 3715	C THR C 158	56.536	14.184	52.517	1.00	23.21	C
	ATOM 3716	O THR C 158	57.338	14.054	51.587	1.00	22.06	O
	ATOM 3717	CB THR C 158	54.606	14.992	51.172	1.00	18.83	C
	ATOM 3718	OG1 THR C 158	53.711	16.090	50.970	1.00	17.97	O
	ATOM 3719	CG2 THR C 158	53.799	13.708	51.280	1.00	17.76	C
	ATOM 3720	N CYS C 159	56.562	13.441	53.617	1.00	26.27	N
	ATOM 3721	CA CYS C 159	57.575	12.421	53.849	1.00	29.55	C
	ATOM 3722	C CYS C 159	57.010	11.001	53.820	1.00	30.89	C
	ATOM 3723	O CYS C 159	56.319	10.581	54.759	1.00	31.67	O
	ATOM 3724	CB CYS C 159	58.260	12.685	55.188	1.00	30.96	C
	ATOM 3725	CG CYS C 159	59.078	14.312	55.287	1.00	34.04	C

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FIG. 53-61

ATOM	3727	CA	THR	C	160	56.825	8.898	52.558	1.00	29.44	C
ATOM	3728	C	THR	C	160	57.966	7.919	52.837	1.00	28.24	C
ATOM	3729	O	THR	C	160	59.019	7.976	52.191	1.00	27.56	O
ATOM	3730	CB	THR	C	160	56.264	8.651	51.130	1.00	30.04	C
ATOM	3731	OG1	THR	C	160	54.997	9.313	50.977	1.00	30.53	O
ATOM	3732	CG2	THR	C	160	56.086	7.167	50.873	1.00	29.78	C
ATOM	3733	N	VAL	C	161	57.763	7.057	53.830	1.00	27.85	N
ATOM	3734	CA	VAL	C	161	58.759	6.056	54.216	1.00	26.29	C
ATOM	3735	C	VAL	C	161	58.402	4.704	53.592	1.00	26.35	C
ATOM	3736	O	VAL	C	161	57.224	4.389	53.402	1.00	25.45	O
ATOM	3737	CB	VAL	C	161	58.849	5.921	55.752	1.00	24.73	C
ATOM	3738	CG1	VAL	C	161	59.797	4.811	56.139	1.00	23.11	C
ATOM	3739	CG2	VAL	C	161	59.325	7.217	56.351	1.00	23.75	C
ATOM	3740	N	LEU	C	162	59.416	3.905	53.288	1.00	25.96	N
ATOM	3741	CA	LEU	C	162	59.188	2.616	52.669	1.00	26.82	C
ATOM	3742	C	LEU	C	162	59.946	1.535	53.421	1.00	26.47	C
ATOM	3743	O	LEU	C	162	61.175	1.589	53.544	1.00	26.00	O
ATOM	3744	CB	LEU	C	162	59.627	2.671	51.199	1.00	29.28	C
ATOM	3745	CG	LEU	C	162	59.135	1.642	50.166	1.00	30.56	C
ATOM	3746	CD1	LEU	C	162	59.208	2.259	48.782	1.00	31.27	C
ATOM	3747	CD2	LEU	C	162	59.943	0.355	50.228	1.00	30.37	C
ATOM	3748	N	GLN	C	163	59.190	0.584	53.961	1.00	26.98	N
ATOM	3749	CA	GLN	C	163	59.721	-0.556	54.711	1.00	26.71	C
ATOM	3750	C	GLN	C	163	58.865	-1.754	54.317	1.00	27.66	C
ATOM	3751	O	GLN	C	163	57.635	-1.667	54.317	1.00	27.62	O
ATOM	3752	CB	GLN	C	163	59.608	-0.315	56.219	1.00	24.98	C
ATOM	3753	CG	GLN	C	163	59.890	-1.540	57.091	1.00	25.25	C
ATOM	3754	CD	GLN	C	163	61.352	-1.980	57.082	1.00	27.07	C
ATOM	3755	OE1	GLN	C	163	62.263	-1.161	56.930	1.00	26.36	O
ATOM	3756	NE2	GLN	C	163	61.583	-3.273	57.276	1.00	27.43	N
ATOM	3757	N	ASN	C	164	59.517	-2.852	53.936	1.00	28.18	N
ATOM	3758	CA	ASN	C	164	58.820	-4.074	53.524	1.00	27.28	C
ATOM	3759	C	ASN	C	164	57.828	-3.806	52.400	1.00	28.24	C
ATOM	3760	O	ASN	C	164	56.665	-4.187	52.499	1.00	27.33	O
ATOM	3761	CB	ASN	C	164	58.061	-4.715	54.697	1.00	25.86	C
ATOM	3762	CG	ASN	C	164	58.962	-5.104	55.844	1.00	23.54	C
ATOM	3763	OD1	ASN	C	164	59.178	-4.324	56.761	1.00	24.92	O
ATOM	3764	ND2	ASN	C	164	59.484	-6.315	55.805	1.00	22.09	N
ATOM	3765	N	GLN	C	165	58.273	-3.108	51.356	1.00	30.69	N
ATOM	3766	CA	GLN	C	165	57.422	-2.815	50.204	1.00	33.45	C
ATOM	3767	C	GLN	C	165	56.179	-2.018	50.597	1.00	34.13	C
ATOM	3768	O	GLN	C	165	55.264	-1.836	49.785	1.00	33.27	O
ATOM	3769	CB	GLN	C	165	57.021	-4.141	49.546	1.00	38.26	C
ATOM	3770	CG	GLN	C	165	56.205	-4.055	48.273	1.00	43.02	C
ATOM	3771	CD	GLN	C	165	55.592	-5.399	47.917	1.00	44.68	C
ATOM	3772	OE1	GLN	C	165	56.250	-6.261	47.335	1.00	45.21	O
ATOM	3773	NE2	GLN	C	165	54.342	-5.600	48.311	1.00	45.67	N
ATOM	3774	N	LYS	C	166	56.159	-1.535	51.839	1.00	35.23	N
ATOM	3775	CA	LYS	C	166	55.040	-0.759	52.371	1.00	35.64	C
ATOM	3776	C	LYS	C	166	55.434	0.697	52.575	1.00	36.20	C
ATOM	3777	O	LYS	C	166	56.621	1.010	52.717	1.00	36.47	O
ATOM	3778	CB	LYS	C	166	54.550	-1.356	53.694	1.00	34.32	C
ATOM	3779	CG	LYS	C	166	53.805	-2.670	53.544	1.00	31.93	C
ATOM	3780	CD	LYS	C	166	52.726	-2.536	52.490	1.00	32.10	C
ATOM	3781	CE	LYS	C	166	51.630	-3.542	52.697	1.00	32.61	C
ATOM	3782	NZ	LYS	C	166	51.076	-3.407	54.073	1.00	35.68	N
ATOM	3783	N	LYS	C	167	54.438	1.582	52.609	1.00	36.33	N
ATOM	3784	CA	LYS	C	167	54.707	3.004	52.776	1.00	35.96	C
ATOM	3785	C	LYS	C	167	53.693	3.782	53.608	1.00	34.21	C
ATOM	3786	O	LYS	C	167	52.486	3.622	53.453	1.00	33.28	O
ATOM	3787	CB	LYS	C	167	54.836	3.690	51.406	1.00	37.91	C
ATOM	3788	CG	LYS	C	167	53.526	3.825	50.623	1.00	41.44	C
ATOM	3789	CD	LYS	C	167	53.272	5.269	50.161	1.00	45.13	C
ATOM	3790	CE	LYS	C	167	52.757	6.171	51.290	1.00	46.91	C
ATOM	3791	NZ	LYS	C	167	52.666	7.622	50.894	1.00	50.08	N
ATOM	3792	N	VAL	C	168	54.207	4.634	54.485	1.00	33.66	N
ATOM	3793	CA	VAL	C	168	53.387	5.508	55.313	1.00	32.71	C
ATOM	3794	C	VAL	C	168	53.762	6.918	54.874	1.00	31.76	C
ATOM	3795	O	VAL	C	168	54.911	7.167	54.477	1.00	30.63	O
ATOM	3796	CB	VAL	C	168	53.642	6.324	55.822	1.00	32.02	C

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FIG. 53-62	ATOM 3798	CG2 VAL C 168	55.129	5.220	57.129	1.00	32.67	C
	ATOM 3799	N GLU C 169	52.779	7.815	54.892	1.00	31.71	N
	ATOM 3800	CA GLU C 169	52.967	9.204	54.469	1.00	30.89	C
	ATOM 3801	C GLU C 169	52.908	10.141	55.670	1.00	29.82	C
	ATOM 3802	O GLU C 169	51.959	10.078	56.463	1.00	29.23	O
	ATOM 3803	CB GLU C 169	51.883	9.560	53.454	1.00	31.18	C
	ATOM 3804	CG GLU C 169	52.069	10.876	52.745	1.00	32.95	C
	ATOM 3805	CD GLU C 169	51.017	11.105	51.684	1.00	32.44	C
	ATOM 3806	OE1 GLU C 169	50.987	10.316	50.716	1.00	36.25	O
	ATOM 3807	OE2 GLU C 169	50.219	12.056	51.821	1.00	31.12	O
	ATOM 3808	N PHE C 170	53.917	11.001	55.790	1.00	28.79	N
	ATOM 3809	CA PHE C 170	54.026	11.952	56.899	1.00	28.29	C
	ATOM 3810	C PHE C 170	54.136	13.396	56.407	1.00	27.47	C
	ATOM 3811	O PHE C 170	55.215	13.836	56.008	1.00	27.61	O
	ATOM 3812	CB PHE C 170	55.281	11.661	57.739	1.00	29.48	C
	ATOM 3813	CG PHE C 170	55.233	10.382	58.518	1.00	29.76	C
	ATOM 3814	CD1 PHE C 170	54.314	10.206	59.550	1.00	30.83	C
	ATOM 3815	CD2 PHE C 170	56.146	9.365	58.257	1.00	30.55	C
	ATOM 3816	CE1 PHE C 170	54.316	9.038	60.318	1.00	30.05	C
	ATOM 3817	CE2 PHE C 170	56.155	8.193	59.020	1.00	30.30	C
	ATOM 3818	CZ PHE C 170	55.236	8.030	60.050	1.00	29.19	C
	ATOM 3819	N LYS C 171	53.042	14.145	56.454	1.00	26.50	N
	ATOM 3820	CA LYS C 171	53.068	15.541	56.026	1.00	25.38	C
	ATOM 3821	C LYS C 171	53.494	16.403	57.213	1.00	24.25	C
	ATOM 3822	O LYS C 171	52.856	16.347	58.260	1.00	25.65	O
	ATOM 3823	CB LYS C 171	51.682	15.954	55.542	1.00	25.88	C
	ATOM 3824	CG LYS C 171	51.206	15.200	54.314	1.00	25.96	C
	ATOM 3825	CD LYS C 171	49.782	15.602	53.942	1.00	28.50	C
	ATOM 3826	CE LYS C 171	49.730	17.011	53.362	1.00	29.70	C
	ATOM 3827	NZ LYS C 171	48.342	17.504	53.122	1.00	29.71	N
	ATOM 3828	N ILE C 172	54.574	17.172	57.071	1.00	22.36	N
	ATOM 3829	CA ILE C 172	55.082	18.024	58.162	1.00	20.16	C
	ATOM 3830	C ILE C 172	55.199	19.493	57.737	1.00	19.90	C
	ATOM 3831	O ILE C 172	55.846	19.803	56.745	1.00	19.88	O
	ATOM 3832	CB ILE C 172	56.491	17.573	58.627	1.00	19.36	C
	ATOM 3833	CG1 ILE C 172	56.653	16.043	58.542	1.00	18.58	C
	ATOM 3834	CG2 ILE C 172	56.745	18.058	60.046	1.00	19.32	C
	ATOM 3835	CD1 ILE C 172	56.013	15.247	59.677	1.00	17.14	C
	ATOM 3836	N ASP C 173	54.640	20.397	58.535	1.00	20.38	N
	ATOM 3837	CA ASP C 173	54.649	21.829	58.230	1.00	19.82	C
	ATOM 3838	C ASP C 173	55.888	22.566	58.698	1.00	19.67	C
	ATOM 3839	O ASP C 173	56.191	22.585	59.888	1.00	19.89	O
	ATOM 3840	CB ASP C 173	53.418	22.513	58.843	1.00	20.41	C
	ATOM 3841	CG ASP C 173	52.123	22.073	58.202	1.00	20.60	C
	ATOM 3842	OD1 ASP C 173	51.725	20.902	58.381	1.00	22.57	O
	ATOM 3843	OD2 ASP C 173	51.496	22.894	57.513	1.00	21.31	O
	ATOM 3844	N ILE C 174	56.582	23.203	57.764	1.00	19.91	N
	ATOM 3845	CA ILE C 174	57.778	23.981	58.075	1.00	19.69	C
	ATOM 3846	C ILE C 174	57.437	25.432	57.737	1.00	18.43	C
	ATOM 3847	O ILE C 174	56.721	25.686	56.762	1.00	17.50	O
	ATOM 3848	CB ILE C 174	58.995	23.580	57.181	1.00	21.54	C
	ATOM 3849	CG1 ILE C 174	59.186	22.061	57.138	1.00	23.72	C
	ATOM 3850	CG2 ILE C 174	60.265	24.227	57.708	1.00	22.56	C
	ATOM 3851	CD1 ILE C 174	59.535	21.423	58.473	1.00	24.97	C
	ATOM 3852	N VAL C 175	57.927	26.379	58.530	1.00	15.80	N
	ATOM 3853	CA VAL C 175	57.672	27.784	58.248	1.00	15.23	C
	ATOM 3854	C VAL C 175	58.984	28.538	58.046	1.00	15.59	C
	ATOM 3855	O VAL C 175	59.722	28.783	58.999	1.00	14.83	O
	ATOM 3856	CB VAL C 175	56.848	28.479	59.367	1.00	15.13	C
	ATOM 3857	CG1 VAL C 175	56.780	29.991	59.118	1.00	11.47	C
	ATOM 3858	CG2 VAL C 175	55.447	27.891	59.438	1.00	13.88	C
	ATOM 3859	N VAL C 176	59.285	28.885	56.802	1.00	15.76	N
	ATOM 3860	CA VAL C 176	60.498	29.637	56.508	1.00	16.89	C
	ATOM 3861	C VAL C 176	60.088	31.109	56.400	1.00	18.51	C
	ATOM 3862	O VAL C 176	59.476	31.537	55.411	1.00	19.47	O
	ATOM 3863	CB VAL C 176	61.148	29.174	55.202	1.00	17.23	C
	ATOM 3864	CG1 VAL C 176	62.568	29.713	55.115	1.00	18.51	C
	ATOM 3865	CG2 VAL C 176	61.133	27.653	55.123	1.00	16.01	C
	ATOM 3866	N LEU C 177	60.374	31.855	57.462	1.00	18.16	N
	ATOM 3867	CA TRP C 177	60.047	33.269	57.577	1.00	17.22	C

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FIG. 53-63	ATOM 3869	O LEU C 177	61.678	33.966	55.944	1.00	17.36	O
	ATOM 3870	CB LEU C 177	60.575	33.798	58.906	1.00	16.95	C
	ATOM 3871	CG LEU C 177	59.568	34.354	59.908	1.00	15.24	C
	ATOM 3872	CD1 LEU C 177	58.294	33.532	59.933	1.00	16.51	C
	ATOM 3873	CD2 LEU C 177	60.212	34.369	61.270	1.00	18.02	C
	ATOM 3874	N ALA C 178	59.722	35.099	56.046	1.00	17.39	N
	ATOM 3875	CA ALA C 178	60.050	36.037	54.981	1.00	18.66	C
	ATOM 3876	C ALA C 178	60.698	37.296	55.555	1.00	19.74	C
	ATOM 3877	O ALA C 178	60.512	37.617	56.731	1.00	19.40	O
	ATOM 3878	CB ALA C 178	58.805	36.389	54.197	1.00	17.39	C
	ATOM 3879	N PHE C 179	61.449	38.007	54.719	1.00	22.31	N
	ATOM 3880	CA PHE C 179	62.136	39.225	55.142	1.00	25.40	C
	ATOM 3881	C PHE C 179	62.398	40.152	53.959	1.00	29.04	C
	ATOM 3882	O PHE C 179	62.740	39.698	52.859	1.00	30.27	O
	ATOM 3883	CB PHE C 179	63.468	38.885	55.803	1.00	23.89	C
	ATOM 3884	CG PHE C 179	64.529	38.418	54.842	1.00	23.56	C
	ATOM 3885	CD1 PHE C 179	64.566	37.103	54.407	1.00	24.11	C
	ATOM 3886	CD2 PHE C 179	65.516	39.292	54.403	1.00	23.56	C
	ATOM 3887	CE1 PHE C 179	65.574	36.661	53.555	1.00	25.53	C
	ATOM 3888	CE2 PHE C 179	66.528	38.857	53.550	1.00	25.32	C
	ATOM 3889	CZ PHE C 179	66.558	37.541	53.127	1.00	24.42	C
	ATOM 3890	N GLN C 180	62.252	41.451	54.188	1.00	31.01	N
	ATOM 3891	CA GLN C 180	62.485	42.428	53.136	1.00	31.97	C
	ATOM 3892	C GLN C 180	63.836	43.125	53.282	1.00	32.39	C
	ATOM 3893	O GLN C 180	64.428	43.146	54.366	1.00	33.39	O
	ATOM 3894	CB GLN C 180	61.353	43.454	53.094	1.00	32.09	C
	ATOM 3895	CG GLN C 180	60.438	43.300	51.897	1.00	33.19	C
	ATOM 3896	CD GLN C 180	61.176	43.467	50.582	1.00	33.40	C
	ATOM 3897	OE1 GLN C 180	62.101	42.717	50.276	1.00	34.04	O
	ATOM 3898	NE2 GLN C 180	60.764	44.445	49.793	1.00	34.51	N
	ATOM 3899	N LYS C 181	64.329	43.661	52.171	1.00	32.34	N
	ATOM 3900	CA LYS C 181	65.603	44.362	52.134	1.00	31.99	C
	ATOM 3901	C LYS C 181	65.577	45.584	53.038	1.00	32.66	C
	ATOM 3902	O LYS C 181	64.692	46.432	52.800	1.00	33.70	O
	ATOM 3903	CB LYS C 181	65.924	44.794	50.698	1.00	31.91	C
	ATOM 3904	CG LYS C 181	66.260	43.655	49.748	1.00	31.31	C
	ATOM 3905	CD LYS C 181	67.506	42.908	50.200	1.00	32.09	C
	ATOM 3906	CE LYS C 181	68.738	43.806	50.183	1.00	33.37	C
	ATOM 3907	NZ LYS C 181	69.879	43.175	50.893	1.00	33.00	N
	TER 3908	LYS C 181						
	ATOM 3909	N GLUL 1	-0.316	8.025	77.827	1.00	31.44	N
	ATOM 3910	CA GLUL 1	-1.773	8.334	77.694	1.00	32.29	C
	ATOM 3911	C GLUL 1	-2.361	8.914	78.981	1.00	30.69	C
	ATOM 3912	O GLUL 1	-3.575	8.928	79.169	1.00	30.35	O
	ATOM 3913	CB GLUL 1	-2.545	7.081	77.275	1.00	34.07	C
	ATOM 3914	CG GLUL 1	-3.795	7.366	76.458	1.00	36.70	C
	ATOM 3915	CD GLUL 1	-4.126	6.250	75.473	1.00	40.14	C
	ATOM 3916	OE1 GLUL 1	-3.560	5.138	75.605	1.00	39.72	O
	ATOM 3917	OE2 GLUL 1	-4.946	6.489	74.554	1.00	41.19	O
	ATOM 3918	N LEUL 2	-1.492	9.391	79.867	1.00	29.92	N
	ATOM 3919	CA LEUL 2	-1.922	9.995	81.128	1.00	28.31	C
	ATOM 3920	C LEUL 2	-2.433	11.410	80.874	1.00	28.41	C
	ATOM 3921	O LEUL 2	-1.743	12.223	80.250	1.00	27.72	O
	ATOM 3922	CB LEUL 2	-0.754	10.058	82.115	1.00	25.05	C
	ATOM 3923	CG LEUL 2	-0.670	9.013	83.225	1.00	23.51	C
	ATOM 3924	CD1 LEUL 2	-1.767	9.288	84.218	1.00	24.46	C
	ATOM 3925	CD2 LEUL 2	-0.759	7.600	82.677	1.00	18.26	C
	ATOM 3926	N GLUL 3	-3.664	11.675	81.297	1.00	28.26	N
	ATOM 3927	CA GLUL 3	-4.249	12.996	81.129	1.00	27.49	C
	ATOM 3928	C GLUL 3	-4.207	13.689	82.485	1.00	26.05	C
	ATOM 3929	O GLUL 3	-4.782	13.202	83.467	1.00	26.90	O
	ATOM 3930	CB GLUL 3	-5.679	12.888	80.606	1.00	28.46	C
	ATOM 3931	CG GLUL 3	-6.274	14.211	80.162	1.00	33.07	C
	ATOM 3932	CD GLUL 3	-7.317	14.733	81.128	1.00	36.39	C
	ATOM 3933	OE1 GLUL 3	-6.982	14.931	82.314	1.00	38.96	O
	ATOM 3934	OE2 GLUL 3	-8.475	14.932	80.703	1.00	36.94	O
	ATOM 3935	N LEUL 4	-3.466	14.788	82.543	1.00	23.66	N
	ATOM 3936	CA LEUL 4	-3.300	15.558	83.768	1.00	20.72	C
	ATOM 3937	C LEUL 4	-4.177	16.809	83.771	1.00	20.47	C
	ATOM 3938	O LEUL 4	-4.431	17.412	82.722	1.00	19.71	O



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FIG. 53-64	ATOM 3940	CG LEUL 4	-0.903	14.698	84.119	1.00	15.50	C
	ATOM 3941	CD1 LEUL 4	0.535	15.079	83.893	1.00	15.51	C
	ATOM 3942	CD2 LEUL 4	-1.073	14.113	85.500	1.00	14.36	C
	ATOM 3943	N THRL 5	-4.646	17.194	84.955	1.00	19.86	N
	ATOM 3944	CA THRL 5	-5.516	18.357	85.093	1.00	19.04	C
	ATOM 3945	C THRL 5	-5.189	19.082	86.373	1.00	19.42	C
	ATOM 3946	O THRL 5	-5.033	18.458	87.420	1.00	21.99	O
	ATOM 3947	CB THRL 5	-7.010	17.958	85.197	1.00	18.26	C
	ATOM 3948	OG1 THRL 5	-7.406	17.182	84.057	1.00	16.67	O
	ATOM 3949	CG2 THRL 5	-7.878	19.197	85.299	1.00	16.92	C
	ATOM 3950	N GLNL 6	-5.085	20.401	86.287	1.00	18.59	N
	ATOM 3951	CA GLNL 6	-4.814	21.221	87.451	1.00	17.69	C
	ATOM 3952	C GLNL 6	-6.155	21.905	87.682	1.00	20.76	C
	ATOM 3953	O GLNL 6	-6.705	22.543	86.779	1.00	19.35	O
	ATOM 3954	CB GLNL 6	-3.667	22.175	87.146	1.00	14.41	C
	ATOM 3955	CG GLNL 6	-2.452	21.397	86.637	1.00	10.06	C
	ATOM 3956	CD GLNL 6	-1.225	22.237	86.407	1.00	7.80	C
	ATOM 3957	OE1 GLNL 6	-0.471	22.015	85.457	1.00	6.57	O
	ATOM 3958	NE2 GLNL 6	-1.007	23.201	87.272	1.00	8.61	N
	ATOM 3959	N SERL 7	-6.724	21.644	88.857	1.00	25.00	N
	ATOM 3960	CA SERL 7	-8.047	22.132	89.245	1.00	27.51	C
	ATOM 3961	C SERL 7	-8.334	23.626	89.169	1.00	27.97	C
	ATOM 3962	O SERL 7	-9.099	24.063	88.300	1.00	30.44	O
	ATOM 3963	CB SERL 7	-8.440	21.547	90.600	1.00	29.38	C
	ATOM 3964	OG SERL 7	-8.318	20.128	90.588	1.00	32.11	O
	ATOM 3965	N PROL 8	-7.754	24.438	90.070	1.00	26.22	N
	ATOM 3966	CA PROL 8	-8.063	25.872	89.949	1.00	24.93	C
	ATOM 3967	C PROL 8	-7.308	26.492	88.758	1.00	24.76	C
	ATOM 3968	O PROL 8	-6.081	26.631	88.790	1.00	24.81	O
	ATOM 3969	CB PROL 8	-7.589	26.428	91.290	1.00	24.11	C
	ATOM 3970	CG PROL 8	-6.386	25.576	91.590	1.00	24.77	C
	ATOM 3971	CD PROL 8	-6.817	24.181	91.180	1.00	24.26	C
	ATOM 3972	N ALAL 9	-8.033	26.814	87.690	1.00	23.55	N
	ATOM 3973	CA ALAL 9	-7.415	27.403	86.502	1.00	21.35	C
	ATOM 3974	C ALAL 9	-6.713	28.709	86.844	1.00	20.25	C
	ATOM 3975	O ALAL 9	-5.674	29.042	86.256	1.00	20.22	O
	ATOM 3976	CB ALAL 9	-8.454	27.630	85.422	1.00	21.24	C
	ATOM 3977	N THRL 10	-7.298	29.453	87.779	1.00	19.33	N
	ATOM 3978	CA THRL 10	-6.742	30.724	88.231	1.00	18.37	C
	ATOM 3979	C THRL 10	-6.945	30.852	89.744	1.00	17.83	C
	ATOM 3980	O THRL 10	-8.058	30.663	90.255	1.00	17.66	O
	ATOM 3981	CB THRL 10	-7.411	31.932	87.524	1.00	19.55	C
	ATOM 3982	OG1 THRL 10	-8.177	31.484	86.393	1.00	21.65	O
	ATOM 3983	CG2 THRL 10	-6.356	32.913	87.050	1.00	17.75	C
	ATOM 3984	N LEUL 11	-5.861	31.118	90.464	1.00	16.23	N
	ATOM 3985	CA LEUL 11	-5.933	31.276	91.907	1.00	15.32	C
	ATOM 3986	C LEUL 11	-5.573	32.720	92.270	1.00	15.02	C
	ATOM 3987	O LEUL 11	-4.500	33.219	91.901	1.00	12.98	O
	ATOM 3988	CB LEUL 11	-4.980	30.308	92.613	1.00	14.18	C
	ATOM 3989	CG LEUL 11	-5.226	30.185	94.115	1.00	13.89	C
	ATOM 3990	CD1 LEUL 11	-6.534	29.461	94.361	1.00	14.46	C
	ATOM 3991	CD2 LEUL 11	-4.086	29.440	94.758	1.00	14.10	C
	ATOM 3992	N SERL 12	-6.479	33.382	92.986	1.00	15.52	N
	ATOM 3993	CA SERL 12	-6.291	34.766	93.398	1.00	15.65	C
	ATOM 3994	C SERL 12	-5.992	34.813	94.893	1.00	16.19	C
	ATOM 3995	O SERL 12	-6.873	34.550	95.718	1.00	17.01	O
	ATOM 3996	CB SERL 12	-7.559	35.573	93.083	1.00	16.63	C
	ATOM 3997	OG SERL 12	-7.962	35.433	91.719	1.00	16.33	O
	ATOM 3998	N VALL 13	-4.758	35.162	95.243	1.00	15.69	N
	ATOM 3999	CA VALL 13	-4.337	35.232	96.642	1.00	15.92	C
	ATOM 4000	C VALL 13	-3.636	36.547	97.008	1.00	15.53	C
	ATOM 4001	O VALL 13	-2.892	37.112	96.207	1.00	14.64	O
	ATOM 4002	CB VALL 13	-3.389	34.059	97.000	1.00	16.50	C
	ATOM 4003	CG1 VALL 13	-4.162	32.750	97.068	1.00	17.04	C
	ATOM 4004	CG2 VALL 13	-2.282	33.949	95.961	1.00	17.84	C
	ATOM 4005	N SERL 14	-3.881	37.029	98.222	1.00	15.24	N
	ATOM 4006	CA SERL 14	-3.265	38.258	98.702	1.00	16.02	C
	ATOM 4007	C SERL 14	-1.807	37.949	99.074	1.00	15.89	C
	ATOM 4008	O SERL 14	-1.534	36.976	99.779	1.00	17.69	O
	ATOM 4009	CB SERL 14	-4.041	38.704	99.007	1.00	17.24	C

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FIG. 53-65

ATOM 4011	N	PROL 15	-0.860	38.810	98.662	1.00	14.23	N
ATOM 4012	CA	PROL 15	0.562	38.602	98.952	1.00	13.05	C
ATOM 4013	C	PROL 15	0.814	38.343	100.423	1.00	13.44	C
ATOM 4014	O	PROL 15	0.259	39.025	101.281	1.00	16.17	O
ATOM 4015	CB	PROL 15	1.196	39.934	98.548	1.00	12.79	C
ATOM 4016	CG	PROL 15	0.226	40.529	97.590	1.00	13.35	C
ATOM 4017	CD	PROL 15	-1.095	40.185	98.191	1.00	13.28	C
ATOM 4018	N	GLYL 16	1.672	37.378	100.711	1.00	12.99	N
ATOM 4019	CA	GLYL 16	2.005	37.070	102.085	1.00	12.12	C
ATOM 4020	C	GLYL 16	1.178	35.955	102.674	1.00	13.08	C
ATOM 4021	O	GLYL 16	1.571	35.374	103.684	1.00	13.68	O
ATOM 4022	N	GLUL 17	0.009	35.706	102.092	1.00	14.80	N
ATOM 4023	CA	GLUL 17	-0.897	34.639	102.533	1.00	15.89	C
ATOM 4024	C	GLUL 17	-0.392	33.287	102.009	1.00	15.65	C
ATOM 4025	O	GLUL 17	0.686	33.215	101.432	1.00	15.62	O
ATOM 4026	CB	GLUL 17	-2.300	34.899	101.975	1.00	16.44	C
ATOM 4027	CG	GLUL 17	-3.380	35.066	103.022	1.00	20.28	C
ATOM 4028	CD	GLUL 17	-3.811	36.507	103.218	1.00	23.46	C
ATOM 4029	OE1	GLUL 17	-3.203	37.410	102.601	1.00	26.76	O
ATOM 4030	OE2	GLUL 17	-4.768	36.747	103.993	1.00	23.58	O
ATOM 4031	N	ARGL 18	-1.199	32.241	102.162	1.00	17.45	N
ATOM 4032	CA	ARGL 18	-0.856	30.892	101.709	1.00	18.54	C
ATOM 4033	C	ARGL 18	-1.681	30.440	100.496	1.00	19.46	C
ATOM 4034	O	ARGL 18	-2.878	30.738	100.409	1.00	21.63	O
ATOM 4035	CB	ARGL 18	-1.064	29.910	102.857	1.00	19.38	C
ATOM 4036	CG	ARGL 18	-1.083	28.442	102.460	1.00	20.71	C
ATOM 4037	CD	ARGL 18	-1.373	27.569	103.660	1.00	20.07	C
ATOM 4038	NE	ARGL 18	-0.260	27.536	104.602	1.00	22.13	N
ATOM 4039	CZ	ARGL 18	0.415	26.431	104.907	1.00	24.21	C
ATOM 4040	NH1	ARGL 18	0.081	25.280	104.331	1.00	23.29	N
ATOM 4041	NH2	ARGL 18	1.405	26.467	105.795	1.00	24.99	N
ATOM 4042	N	ALAL 19	-1.049	29.683	99.595	1.00	18.65	N
ATOM 4043	CA	ALAL 19	-1.702	29.155	98.378	1.00	16.57	C
ATOM 4044	C	ALAL 19	-1.544	27.629	98.196	1.00	13.56	C
ATOM 4045	O	ALAL 19	-0.500	27.060	98.496	1.00	11.67	O
ATOM 4046	CB	ALAL 19	-1.173	29.883	97.145	1.00	14.46	C
ATOM 4047	N	THRL 20	-2.584	26.980	97.688	1.00	12.77	N
ATOM 4048	CA	THRL 20	-2.573	25.535	97.463	1.00	12.50	C
ATOM 4049	C	THRL 20	-3.238	25.158	96.137	1.00	11.49	C
ATOM 4050	O	THRL 20	-4.430	25.411	95.946	1.00	11.49	O
ATOM 4051	CB	THRL 20	-3.259	24.789	98.646	1.00	12.82	C
ATOM 4052	OG1	THRL 20	-2.272	24.409	99.619	1.00	12.71	O
ATOM 4053	CG2	THRL 20	-4.023	23.559	98.164	1.00	13.86	C
ATOM 4054	N	LEUL 21	-2.471	24.522	95.250	1.00	11.90	N
ATOM 4055	CA	LEUL 21	-2.952	24.106	93.923	1.00	13.41	C
ATOM 4056	C	LEUL 21	-3.006	22.580	93.754	1.00	15.85	C
ATOM 4057	O	LEUL 21	-2.062	21.877	94.114	1.00	16.34	O
ATOM 4058	CB	LEUL 21	-2.038	24.673	92.838	1.00	10.60	C
ATOM 4059	CG	LEUL 21	-1.291	25.990	93.057	1.00	9.16	C
ATOM 4060	CD1	LEUL 21	-0.495	26.310	91.801	1.00	7.83	C
ATOM 4061	CD2	LEUL 21	-2.243	27.113	93.366	1.00	8.13	C
ATOM 4062	N	SERL 22	-4.072	22.079	93.134	1.00	17.86	N
ATOM 4063	CA	SERL 22	-4.234	20.639	92.927	1.00	18.46	C
ATOM 4064	C	SERL 22	-4.021	20.166	91.491	1.00	18.18	C
ATOM 4065	O	SERL 22	-4.403	20.849	90.532	1.00	18.53	O
ATOM 4066	CB	SERL 22	-5.611	20.184	93.423	1.00	20.56	C
ATOM 4067	OG	SERL 22	-6.650	21.002	92.910	1.00	22.97	O
ATOM 4068	N	CYSL 23	-3.460	18.967	91.356	1.00	17.73	N
ATOM 4069	CA	CYSL 23	-3.176	18.355	90.059	1.00	17.22	C
ATOM 4070	C	CYSL 23	-3.592	16.886	90.057	1.00	18.28	C
ATOM 4071	O	CYSL 23	-2.934	16.042	90.680	1.00	19.49	O
ATOM 4072	CB	CYSL 23	-1.685	18.459	89.760	1.00	16.10	C
ATOM 4073	SG	CYSL 23	-1.058	17.315	88.491	1.00	15.24	S
ATOM 4074	N	ARGL 24	-4.701	16.589	89.390	1.00	17.66	N
ATOM 4075	CA	ARGL 24	-5.201	15.227	89.308	1.00	19.01	C
ATOM 4076	C	ARGL 24	-4.729	14.531	88.026	1.00	19.38	C
ATOM 4077	O	ARGL 24	-4.286	15.191	87.079	1.00	19.33	O
ATOM 4078	CB	ARGL 24	-6.741	15.235	89.389	1.00	21.08	C
ATOM 4079	CG	ARGL 24	-7.483	14.343	88.364	1.00	21.37	C
ATOM 4080	CD	ARGL 24	-8.101	15.175	87.738	1.00	23.45	C

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FIG. 53-66	ATOM 4082 CZ ARGL 24	-8.028	13.949	85.105	1.00	21.21	C
	ATOM 4083 NH1 ARGL 24	-6.747	14.265	84.949	1.00	18.73	N
	ATOM 4084 NH2 ARGL 24	-8.646	13.226	84.177	1.00	21.96	N
	ATOM 4085 N ALAL 25	-4.842	13.202	88.008	1.00	19.40	N
	ATOM 4086 CA ALAL 25	-4.486	12.376	86.854	1.00	18.37	C
	ATOM 4087 C ALAL 25	-5.646	11.409	86.562	1.00	18.52	C
	ATOM 4088 O ALAL 25	-6.455	11.108	87.444	1.00	18.35	O
	ATOM 4089 CB ALAL 25	-3.209	11.608	87.127	1.00	15.31	C
	ATOM 4090 N SERL 26	-5.765	10.977	85.311	1.00	19.56	N
	ATOM 4091 CA SERL 26	-6.826	10.051	84.899	1.00	19.32	C
	ATOM 4092 C SERL 26	-6.446	8.609	85.202	1.00	20.08	C
	ATOM 4093 O SERL 26	-7.300	7.734	85.293	1.00	19.11	O
	ATOM 4094 CB SERL 26	-7.099	10.202	83.400	1.00	19.52	C
	ATOM 4095 OG SERL 26	-5.890	10.143	82.650	1.00	19.21	O
	ATOM 4096 N GLUL 27	-5.149	8.383	85.369	1.00	21.48	N
	ATOM 4097 CA GLUL 27	-4.606	7.062	85.651	1.00	22.68	C
	ATOM 4098 C GLUL 27	-3.615	7.299	86.784	1.00	21.55	C
	ATOM 4099 O GLUL 27	-3.297	8.449	87.075	1.00	20.70	O
	ATOM 4100 CB GLUL 27	-3.894	6.538	84.397	1.00	24.20	C
	ATOM 4101 CG GLUL 27	-3.422	5.100	84.464	1.00	26.70	C
	ATOM 4102 CD GLUL 27	-2.802	4.629	83.161	1.00	28.70	C
	ATOM 4103 OE1 GLUL 27	-3.303	5.005	82.077	1.00	26.39	O
	ATOM 4104 OE2 GLUL 27	-1.808	3.875	83.223	1.00	31.38	O
	ATOM 4105 N SERL 28	-3.131	6.239	87.430	1.00	20.23	N
	ATOM 4106 CA SERL 28	-2.190	6.431	88.526	1.00	18.82	C
	ATOM 4107 C SERL 28	-0.789	6.746	88.030	1.00	19.09	C
	ATOM 4108 O SERL 28	-0.262	6.066	87.145	1.00	17.76	O
	ATOM 4109 CB SERL 28	-2.153	5.229	89.460	1.00	18.00	C
	ATOM 4110 OG SERL 28	-1.426	5.543	90.645	1.00	14.69	O
	ATOM 4111 N VALL 29	-0.199	7.768	88.650	1.00	18.80	N
	ATOM 4112 CA VALL 29	1.135	8.266	88.334	1.00	17.92	C
	ATOM 4113 C VALL 29	2.209	7.771	89.324	1.00	17.57	C
	ATOM 4114 O VALL 29	3.407	7.919	89.092	1.00	15.94	O
	ATOM 4115 CB VALL 29	1.094	9.814	88.277	1.00	18.83	C
	ATOM 4116 CG1 VALL 29	2.479	10.388	88.093	1.00	20.20	C
	ATOM 4117 CG2 VALL 29	0.178	10.268	87.154	1.00	16.01	C
	ATOM 4118 N SERL 30	1.757	7.238	90.451	1.00	19.43	N
	ATOM 4119 CA SERL 30	2.621	6.680	91.493	1.00	21.15	C
	ATOM 4120 C SERL 30	3.892	7.446	91.899	1.00	22.67	C
	ATOM 4121 O SERL 30	4.993	6.888	91.885	1.00	24.62	O
	ATOM 4122 CB SERL 30	2.963	5.228	91.136	1.00	21.43	C
	ATOM 4123 OG SERL 30	3.696	4.586	92.164	1.00	24.65	O
	ATOM 4124 N SERL 31	3.728	8.694	92.330	1.00	21.72	N
	ATOM 4125 CA SERL 31	4.843	9.535	92.787	1.00	21.00	C
	ATOM 4126 C SERL 31	5.684	10.211	91.715	1.00	20.70	C
	ATOM 4127 O SERL 31	6.423	11.155	92.020	1.00	20.56	O
	ATOM 4128 CB SERL 31	5.766	8.798	93.773	1.00	20.26	C
	ATOM 4129 OG SERL 31	5.092	8.474	94.979	1.00	17.50	O
	ATOM 4130 N ASPL 32	5.569	9.756	90.471	1.00	18.99	N
	ATOM 4131 CA ASPL 32	6.321	10.372	89.383	1.00	16.73	C
	ATOM 4132 C ASPL 32	5.619	11.645	88.924	1.00	15.84	C
	ATOM 4133 O ASPL 32	5.078	11.708	87.820	1.00	16.03	O
	ATOM 4134 CB ASPL 32	6.493	9.389	88.228	1.00	15.22	C
	ATOM 4135 CG ASPL 32	7.479	8.293	88.548	1.00	14.08	C
	ATOM 4136 OD1 ASPL 32	8.686	8.593	88.640	1.00	14.00	O
	ATOM 4137 OD2 ASPL 32	7.052	7.134	88.732	1.00	14.42	O
	ATOM 4138 N LEUL 33	5.616	12.651	89.797	1.00	16.26	N
	ATOM 4139 CA LEUL 33	4.978	13.942	89.524	1.00	14.57	C
	ATOM 4140 C LEUL 33	5.983	15.063	89.770	1.00	13.42	C
	ATOM 4141 O LEUL 33	6.844	14.963	90.649	1.00	14.25	O
	ATOM 4142 CB LEUL 33	3.760	14.134	90.427	1.00	13.78	C
	ATOM 4143 CG LEUL 33	2.706	15.210	90.099	1.00	14.95	C
	ATOM 4144 CD1 LEUL 33	3.156	16.597	90.519	1.00	12.91	C
	ATOM 4145 CD2 LEUL 33	2.326	15.161	88.633	1.00	12.22	C
	ATOM 4146 N ALAL 34	5.877	16.121	88.978	1.00	11.33	N
	ATOM 4147 CA ALAL 34	6.769	17.253	89.086	1.00	6.84	C
	ATOM 4148 C ALAL 34	5.959	18.532	89.121	1.00	6.22	C
	ATOM 4149 O ALAL 34	4.767	18.528	88.809	1.00	7.58	O
	ATOM 4150 CB ALAL 34	7.697	17.262	87.908	1.00	5.43	C
	ATOM 4151 N TDDI 35	6.603	10.625	80.514	1.00	5.26	N

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FIG. 53-67

ATOM 4153 C TRPL 35	6.924	21.966	89.048	1.00	3.47	C
ATOM 4154 O TRPL 35	8.061	22.052	89.515	1.00	3.50	O
ATOM 4155 CB TRPL 35	5.556	21.265	90.997	1.00	5.12	C
ATOM 4156 CG TRPL 35	4.297	20.596	91.453	1.00	4.90	C
ATOM 4157 CD1 TRPL 35	4.195	19.500	92.251	1.00	4.38	C
ATOM 4158 CD2 TRPL 35	2.954	21.036	91.202	1.00	3.51	C
ATOM 4159 NE1 TRPL 35	2.879	19.238	92.524	1.00	2.89	N
ATOM 4160 CE2 TRPL 35	2.099	20.163	91.895	1.00	2.00	C
ATOM 4161 CE3 TRPL 35	2.400	22.083	90.464	1.00	3.91	C
ATOM 4162 CZ2 TRPL 35	0.718	20.312	91.876	1.00	2.00	C
ATOM 4163 CZ3 TRPL 35	1.021	22.228	90.448	1.00	2.00	C
ATOM 4164 CH2 TRPL 35	0.198	21.347	91.149	1.00	2.38	C
ATOM 4165 N TYRL 36	6.470	22.740	88.064	1.00	4.17	N
ATOM 4166 CA TYRL 36	7.281	23.779	87.440	1.00	4.96	C
ATOM 4167 C TYRL 36	6.663	25.180	87.538	1.00	6.14	C
ATOM 4168 O TYRL 36	5.444	25.349	87.467	1.00	7.01	O
ATOM 4169 CB TYRL 36	7.525	23.442	85.973	1.00	3.09	C
ATOM 4170 CG TYRL 36	8.077	22.057	85.749	1.00	2.00	C
ATOM 4171 CD1 TYRL 36	7.225	20.951	85.671	1.00	2.93	C
ATOM 4172 CD2 TYRL 36	9.441	21.848	85.616	1.00	2.00	C
ATOM 4173 CE1 TYRL 36	7.726	19.676	85.468	1.00	2.08	C
ATOM 4174 CE2 TYRL 36	9.953	20.585	85.415	1.00	2.34	C
ATOM 4175 CZ TYRL 36	9.094	19.497	85.343	1.00	3.39	C
ATOM 4176 OH TYRL 36	9.610	18.233	85.179	1.00	2.55	O
ATOM 4177 N GLNL 37	7.520	26.178	87.696	1.00	5.95	N
ATOM 4178 CA GLNL 37	7.087	27.554	87.792	1.00	5.78	C
ATOM 4179 C GLNL 37	7.510	28.300	86.531	1.00	5.25	C
ATOM 4180 O GLNL 37	8.668	28.219	86.101	1.00	4.79	O
ATOM 4181 CB GLNL 37	7.728	28.216	89.016	1.00	6.32	C
ATOM 4182 CG GLNL 37	7.256	29.643	89.288	1.00	5.43	C
ATOM 4183 CD GLNL 37	8.156	30.369	90.261	1.00	4.23	C
ATOM 4184 OE1 GLNL 37	9.372	30.468	90.052	1.00	4.94	O
ATOM 4185 NE2 GLNL 37	7.569	30.901	91.317	1.00	2.38	N
ATOM 4186 N GLNL 38	6.590	29.018	85.915	1.00	4.82	N
ATOM 4187 CA GLNL 38	6.985	29.751	84.735	1.00	8.35	C
ATOM 4188 C GLNL 38	6.568	31.212	84.803	1.00	11.67	C
ATOM 4189 O GLNL 38	5.398	31.524	85.033	1.00	12.90	O
ATOM 4190 CB GLNL 38	6.451	29.101	83.452	1.00	7.29	C
ATOM 4191 CG GLNL 38	7.234	29.536	82.224	1.00	4.57	C
ATOM 4192 CD GLNL 38	6.624	29.084	80.933	1.00	3.14	C
ATOM 4193 OE1 GLNL 38	5.463	28.700	80.893	1.00	3.34	O
ATOM 4194 NE2 GLNL 38	7.395	29.148	79.858	1.00	2.00	N
ATOM 4195 N LYSL 39	7.552	32.097	84.685	1.00	12.62	N
ATOM 4196 CA LYSL 39	7.288	33.518	84.681	1.00	15.30	C
ATOM 4197 C LYSL 39	6.991	33.778	83.210	1.00	18.12	C
ATOM 4198 O LYSL 39	7.361	32.962	82.364	1.00	20.22	O
ATOM 4199 CB LYSL 39	8.529	34.282	85.130	1.00	15.46	C
ATOM 4200 CG LYSL 39	8.514	34.709	86.599	1.00	16.47	C
ATOM 4201 CD LYSL 39	8.613	33.536	87.561	1.00	16.42	C
ATOM 4202 CE LYSL 39	8.373	33.963	89.012	1.00	14.98	C
ATOM 4203 NZ LYSL 39	9.384	34.893	89.580	1.00	12.96	N
ATOM 4204 N PROL 40	6.337	34.906	82.874	1.00	19.22	N
ATOM 4205 CA PROL 40	6.002	35.242	81.487	1.00	20.79	C
ATOM 4206 C PROL 40	6.847	34.650	80.340	1.00	21.94	C
ATOM 4207 O PROL 40	6.514	33.568	79.823	1.00	23.08	O
ATOM 4208 CB PROL 40	5.991	36.764	81.517	1.00	19.24	C
ATOM 4209 CG PROL 40	5.262	37.005	82.793	1.00	18.51	C
ATOM 4210 CD PROL 40	5.879	35.983	83.773	1.00	18.75	C
ATOM 4211 N GLYL 41	7.893	35.356	79.911	1.00	21.06	N
ATOM 4212 CA GLYL 41	8.712	34.847	78.820	1.00	20.00	C
ATOM 4213 C GLYL 41	9.974	34.121	79.261	1.00	18.97	C
ATOM 4214 O GLYL 41	11.030	34.252	78.633	1.00	19.04	O
ATOM 4215 N GLNL 42	9.874	33.335	80.326	1.00	16.60	N
ATOM 4216 CA GLNL 42	11.032	32.612	80.836	1.00	14.53	C
ATOM 4217 C GLNL 42	10.845	31.084	80.820	1.00	12.62	C
ATOM 4218 O GLNL 42	9.736	30.585	80.996	1.00	11.29	O
ATOM 4219 CB GLNL 42	11.320	33.048	82.270	1.00	16.46	C
ATOM 4220 CG GLNL 42	11.589	34.524	82.496	1.00	15.62	C
ATOM 4221 CD GLNL 42	12.004	34.799	83.937	1.00	16.42	C
ATOM 4222 OE1 GLNL 42	12.068	33.896	84.756	1.00	14.50	O

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FIG. 53-68	ATOM 4224	N	ALAL 43	11.934	30.348	80.614	1.00	11.24	N
	ATOM 4225	CA	ALAL 43	11.905	28.890	80.620	1.00	11.00	C
	ATOM 4226	C	ALAL 43	11.442	28.460	82.005	1.00	12.34	C
	ATOM 4227	O	ALAL 43	11.689	29.172	82.987	1.00	13.78	O
	ATOM 4228	CB	ALAL 43	13.272	28.361	80.353	1.00	12.18	C
	ATOM 4229	N	PROL 44	10.734	27.316	82.110	1.00	13.30	N
	ATOM 4230	CA	PROL 44	10.233	26.818	83.404	1.00	11.61	C
	ATOM 4231	C	PROL 44	11.269	26.510	84.486	1.00	11.74	C
	ATOM 4232	O	PROL 44	12.406	26.119	84.199	1.00	10.92	O
	ATOM 4233	CB	PROL 44	9.441	25.573	83.008	1.00	10.31	C
	ATOM 4234	CG	PROL 44	8.920	25.933	81.645	1.00	9.78	C
	ATOM 4235	CD	PROL 44	10.157	26.534	80.999	1.00	11.64	C
	ATOM 4236	N	ARGL 45	10.844	26.691	85.732	1.00	12.04	N
	ATOM 4237	CA	ARGL 45	11.670	26.450	86.911	1.00	12.58	C
	ATOM 4238	C	ARGL 45	11.185	25.191	87.614	1.00	10.42	C
	ATOM 4239	O	ARGL 45	10.041	25.152	88.059	1.00	10.54	O
	ATOM 4240	CB	ARGL 45	11.556	27.630	87.886	1.00	15.44	C
	ATOM 4241	CG	ARGL 45	12.550	28.760	87.653	1.00	20.75	C
	ATOM 4242	CD	ARGL 45	12.054	30.115	88.218	1.00	24.56	C
	ATOM 4243	NE	ARGL 45	11.048	30.748	87.355	1.00	21.85	N
	ATOM 4244	CZ	ARGL 45	11.279	31.154	86.104	1.00	21.74	C
	ATOM 4245	NH1	ARGL 45	12.486	31.009	85.562	1.00	22.07	N
	ATOM 4246	NH2	ARGL 45	10.289	31.651	85.368	1.00	19.12	N
	ATOM 4247	N	LEUL 46	12.049	24.175	87.709	1.00	8.36	N
	ATOM 4248	CA	LEUL 46	11.729	22.908	88.383	1.00	6.60	C
	ATOM 4249	C	LEUL 46	11.710	23.168	89.877	1.00	5.39	C
	ATOM 4250	O	LEUL 46	12.744	23.503	90.454	1.00	6.29	O
	ATOM 4251	CB	LEUL 46	12.797	21.844	88.064	1.00	6.01	C
	ATOM 4252	CG	LEUL 46	12.724	20.370	88.525	1.00	4.44	C
	ATOM 4253	CD1	LEUL 46	13.724	20.103	89.626	1.00	3.32	C
	ATOM 4254	CD2	LEUL 46	11.315	19.935	88.934	1.00	2.00	C
	ATOM 4255	N	LEUL 47	10.539	23.061	90.491	1.00	4.03	N
	ATOM 4256	CA	LEUL 47	10.425	23.301	91.925	1.00	4.61	C
	ATOM 4257	C	LEUL 47	10.514	22.005	92.699	1.00	6.13	C
	ATOM 4258	O	LEUL 47	11.352	21.858	93.593	1.00	6.17	O
	ATOM 4259	CB	LEUL 47	9.086	23.961	92.271	1.00	4.58	C
	ATOM 4260	CG	LEUL 47	8.644	25.279	91.630	1.00	4.25	C
	ATOM 4261	CD1	LEUL 47	7.228	25.577	92.075	1.00	2.00	C
	ATOM 4262	CD2	LEUL 47	9.598	26.419	91.994	1.00	2.00	C
	ATOM 4263	N	ILEL 48	9.664	21.054	92.315	1.00	6.44	N
	ATOM 4264	CA	ILEL 48	9.568	19.765	92.976	1.00	6.45	C
	ATOM 4265	C	ILEL 48	9.521	18.596	92.000	1.00	6.63	C
	ATOM 4266	O	ILEL 48	9.113	18.740	90.850	1.00	8.77	O
	ATOM 4267	CB	ILEL 48	8.314	19.764	93.888	1.00	6.82	C
	ATOM 4268	CG1	ILEL 48	8.553	20.714	95.067	1.00	6.46	C
	ATOM 4269	CG2	ILEL 48	7.972	18.362	94.372	1.00	6.08	C
	ATOM 4270	CD1	ILEL 48	7.345	21.008	95.869	1.00	6.38	C
	ATOM 4271	N	TYRL 49	9.996	17.444	92.447	1.00	7.79	N
	ATOM 4272	CA	TYRL 49	9.996	16.239	91.628	1.00	7.34	C
	ATOM 4273	C	TYRL 49	9.713	15.065	92.546	1.00	7.29	C
	ATOM 4274	O	TYRL 49	9.787	15.203	93.763	1.00	8.88	O
	ATOM 4275	CB	TYRL 49	11.339	16.061	90.913	1.00	7.81	C
	ATOM 4276	CG	TYRL 49	12.570	15.984	91.799	1.00	8.07	C
	ATOM 4277	CD1	TYRL 49	13.168	17.138	92.307	1.00	8.64	C
	ATOM 4278	CD2	TYRL 49	13.170	14.757	92.079	1.00	8.05	C
	ATOM 4279	CE1	TYRL 49	14.340	17.065	93.069	1.00	9.99	C
	ATOM 4280	CE2	TYRL 49	14.336	14.672	92.836	1.00	7.16	C
	ATOM 4281	CZ	TYRL 49	14.916	15.822	93.324	1.00	8.26	C
	ATOM 4282	OH	TYRL 49	16.085	15.714	94.042	1.00	10.59	O
	ATOM 4283	N	GLYL 50	9.365	13.924	91.977	1.00	5.39	N
	ATOM 4284	CA	GLYL 50	9.081	12.776	92.804	1.00	6.74	C
	ATOM 4285	C	GLYL 50	7.983	13.111	93.787	1.00	8.89	C
	ATOM 4286	O	GLYL 50	8.031	12.720	94.954	1.00	8.92	O
	ATOM 4287	N	ALAL 51	7.034	13.917	93.324	1.00	10.14	N
	ATOM 4288	CA	ALAL 51	5.884	14.344	94.110	1.00	9.53	C
	ATOM 4289	C	ALAL 51	6.142	15.215	95.337	1.00	10.33	C
	ATOM 4290	O	ALAL 51	5.328	16.085	95.639	1.00	11.66	O
	ATOM 4291	CB	ALAL 51	5.045	13.155	94.496	1.00	7.73	C
	ATOM 4292	N	SERL 52	7.276	15.049	96.010	1.00	9.61	N
	ATOM 4293	CA	SERL 52	7.512	15.811	97.778	1.00	9.03	C

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FIG. 53-69	ATOM 4295 O SER L 52	9.137 16.985 98.518 1.00 13.47	O
	ATOM 4296 CB SER L 52	7.048 14.980 98.425 1.00 8.86	C
	ATOM 4297 OG SER L 52	7.734 13.737 98.471 1.00 6.01	O
	ATOM 4298 N THRL 53	9.903 15.951 96.691 1.00 12.37	N
	ATOM 4299 CA THRL 53	11.255 16.428 96.937 1.00 12.97	C
	ATOM 4300 C THRL 53	11.543 17.688 96.142 1.00 15.00	C
	ATOM 4301 O THRL 53	11.422 17.713 94.909 1.00 16.56	O
	ATOM 4302 CB THRL 53	12.311 15.367 96.662 1.00 12.15	C
	ATOM 4303 OG1 THRL 53	13.615 15.951 96.785 1.00 13.42	O
	ATOM 4304 CG2 THRL 53	12.148 14.802 95.294 1.00 13.58	C
	ATOM 4305 N ARGL 54	11.926 18.732 96.867 1.00 16.83	N
	ATOM 4306 CA ARGL 54	12.213 20.044 96.295 1.00 16.86	C
	ATOM 4307 C ARGL 54	13.607 20.133 95.664 1.00 16.76	C
	ATOM 4308 O ARGL 54	14.566 19.549 96.184 1.00 15.87	O
	ATOM 4309 CB ARGL 54	12.047 21.109 97.386 1.00 17.06	C
	ATOM 4310 CG ARGL 54	10.812 20.896 98.265 1.00 17.51	C
	ATOM 4311 CD ARGL 54	10.489 22.113 99.138 1.00 18.35	C
	ATOM 4312 NE ARGL 54	11.659 22.614 99.851 1.00 18.71	N
	ATOM 4313 CZ ARGL 54	12.000 22.248 101.083 1.00 19.95	C
	ATOM 4314 NH1 ARGL 54	11.249 21.382 101.753 1.00 18.43	N
	ATOM 4315 NH2 ARGL 54	13.118 22.717 101.629 1.00 21.61	N
	ATOM 4316 N ALAL 55	13.715 20.903 94.580 1.00 16.45	N
	ATOM 4317 CA ALAL 55	14.971 21.088 93.856 1.00 17.53	C
	ATOM 4318 C ALAL 55	15.933 22.082 94.507 1.00 18.92	C
	ATOM 4319 O ALAL 55	15.517 22.957 95.273 1.00 17.92	O
	ATOM 4320 CB ALAL 55	14.691 21.498 92.440 1.00 18.04	C
	ATOM 4321 N THRL 56	17.219 21.947 94.176 1.00 20.30	N
	ATOM 4322 CA THRL 56	18.286 22.794 94.714 1.00 21.70	C
	ATOM 4323 C THRL 56	18.025 24.293 94.587 1.00 22.13	C
	ATOM 4324 O THRL 56	18.134 24.860 93.500 1.00 21.81	O
	ATOM 4325 CB THRL 56	19.621 22.508 94.026 1.00 21.97	C
	ATOM 4326 OG1 THRL 56	19.713 21.118 93.694 1.00 25.18	O
	ATOM 4327 CG2 THRL 56	20.754 22.855 94.967 1.00 24.12	C
	ATOM 4328 N GLYL 57	17.714 24.935 95.707 1.00 23.10	N
	ATOM 4329 CA GLYL 57	17.451 26.366 95.686 1.00 22.60	C
	ATOM 4330 C GLYL 57	15.966 26.683 95.597 1.00 22.62	C
	ATOM 4331 O GLYL 57	15.564 27.684 94.998 1.00 23.70	O
	ATOM 4332 N VALL 58	15.148 25.816 96.183 1.00 20.52	N
	ATOM 4333 CA VALL 58	13.708 25.988 96.196 1.00 19.52	C
	ATOM 4334 C VALL 58	13.258 26.056 97.651 1.00 20.36	C
	ATOM 4335 O VALL 58	13.203 25.036 98.347 1.00 19.75	O
	ATOM 4336 CB VALL 58	12.995 24.814 95.479 1.00 19.08	C
	ATOM 4337 CG1 VALL 58	11.481 24.943 95.606 1.00 19.49	C
	ATOM 4338 CG2 VALL 58	13.389 24.784 94.016 1.00 18.19	C
	ATOM 4339 N PROL 59	12.967 27.270 98.142 1.00 21.45	N
	ATOM 4340 CA PROL 59	12.518 27.550 99.507 1.00 21.92	C
	ATOM 4341 C PROL 59	11.521 26.544 100.071 1.00 21.94	C
	ATOM 4342 O PROL 59	10.726 25.962 99.333 1.00 21.19	O
	ATOM 4343 CB PROL 59	11.887 28.926 99.360 1.00 22.93	C
	ATOM 4344 CG PROL 59	12.837 29.589 98.409 1.00 22.27	C
	ATOM 4345 CD PROL 59	13.072 28.519 97.364 1.00 22.63	C
	ATOM 4346 N ALAL 60	11.554 26.374 101.394 1.00 22.13	N
	ATOM 4347 CA ALAL 60	10.650 25.459 102.094 1.00 21.74	C
	ATOM 4348 C ALAL 60	9.198 25.902 101.955 1.00 20.47	C
	ATOM 4349 O ALAL 60	8.275 25.168 102.293 1.00 21.56	O
	ATOM 4350 CB ALAL 60	11.030 25.378 103.545 1.00 23.21	C
	ATOM 4351 N ARGL 61	9.041 27.139 101.498 1.00 20.42	N
	ATOM 4352 CA ARGL 61	7.772 27.810 101.243 1.00 19.06	C
	ATOM 4353 C ARGL 61	6.911 26.895 100.364 1.00 17.94	C
	ATOM 4354 O ARGL 61	5.745 26.638 100.664 1.00 18.58	O
	ATOM 4355 CB ARGL 61	8.098 29.103 100.482 1.00 19.44	C
	ATOM 4356 CG ARGL 61	7.048 30.198 100.445 1.00 19.13	C
	ATOM 4357 CD ARGL 61	7.504 31.296 99.459 1.00 19.17	C
	ATOM 4358 NE ARGL 61	8.918 31.648 99.626 1.00 17.54	N
	ATOM 4359 CZ ARGL 61	9.615 32.411 98.787 1.00 17.27	C
	ATOM 4360 NH1 ARGL 61	9.038 32.924 97.712 1.00 17.58	N
	ATOM 4361 NH2 ARGL 61	10.909 32.633 99.002 1.00 16.55	N
	ATOM 4362 N PHEL 62	7.499 26.432 99.266 1.00 16.61	N
	ATOM 4363 CA PHEL 62	6.822 25.548 98.327 1.00 14.88	C
	ATOM 4364 C PHEL 62	6.977 24.140 98.933 1.00 14.11	C

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FIG. 53-70	ATOM 4366 CB PHE L 62	7.561	25.540	96.980	1.00	14.31	C
	ATOM 4367 CG PHE L 62	7.537	26.862	96.236	1.00	10.40	C
	ATOM 4368 CD1 PHE L 62	8.529	27.816	96.445	1.00	9.61	C
	ATOM 4369 CD2 PHE L 62	6.577	27.112	95.259	1.00	8.67	C
	ATOM 4370 CE1 PHE L 62	8.567	28.994	95.684	1.00	8.08	C
	ATOM 4371 CE2 PHE L 62	6.610	28.288	94.496	1.00	7.13	C
	ATOM 4372 CZ PHE L 62	7.607	29.224	94.711	1.00	6.12	C
	ATOM 4373 N SER L 63	5.796	23.388	98.805	1.00	12.89	N
	ATOM 4374 CA SER L 63	5.754	22.033	99.342	1.00	12.61	C
	ATOM 4375 C SER L 63	4.981	21.124	98.419	1.00	12.96	C
	ATOM 4376 O SER L 63	3.998	21.550	97.811	1.00	13.82	O
	ATOM 4377 CB SER L 63	5.117	22.008	100.736	1.00	14.31	C
	ATOM 4378 OG SER L 63	6.075	22.307	101.739	1.00	17.32	O
	ATOM 4379 N GLY L 64	5.445	19.880	98.303	1.00	13.07	N
	ATOM 4380 CA GLY L 64	4.799	18.906	97.447	1.00	11.80	C
	ATOM 4381 C GLY L 64	4.228	17.755	98.243	1.00	11.55	C
	ATOM 4382 O GLY L 64	4.915	17.176	99.087	1.00	11.72	O
	ATOM 4383 N SER L 65	2.974	17.413	97.974	1.00	11.43	N
	ATOM 4384 CA SER L 65	2.318	16.323	98.674	1.00	12.21	C
	ATOM 4385 C SER L 65	1.425	15.520	97.738	1.00	11.84	C
	ATOM 4386 O SER L 65	1.031	16.008	96.672	1.00	10.30	O
	ATOM 4387 CB SER L 65	1.471	16.889	99.808	1.00	13.44	C
	ATOM 4388 OG SER L 65	0.446	17.714	99.286	1.00	17.96	O
	ATOM 4389 N GLY L 66	1.119	14.290	98.143	1.00	12.20	N
	ATOM 4390 CA GLY L 66	0.236	13.441	97.361	1.00	13.58	C
	ATOM 4391 C GLY L 66	0.816	12.286	96.565	1.00	13.54	C
	ATOM 4392 O GLY L 66	2.008	12.247	96.254	1.00	13.29	O
	ATOM 4393 N SER L 67	-0.062	11.358	96.196	1.00	14.26	N
	ATOM 4394 CA SER L 67	0.324	10.185	95.423	1.00	13.93	C
	ATOM 4395 C SER L 67	-0.850	9.651	94.600	1.00	14.21	C
	ATOM 4396 O SER L 67	-1.990	10.099	94.756	1.00	12.98	O
	ATOM 4397 CB SER L 67	0.870	9.097	96.354	1.00	13.59	C
	ATOM 4398 OG SER L 67	0.004	8.866	97.452	1.00	14.62	O
	ATOM 4399 N GLY L 68	-0.561	8.702	93.713	1.00	15.44	N
	ATOM 4400 CA GLY L 68	-1.598	8.117	92.891	1.00	15.85	C
	ATOM 4401 C GLY L 68	-2.062	9.061	91.802	1.00	17.29	C
	ATOM 4402 O GLY L 68	-1.300	9.356	90.876	1.00	17.46	O
	ATOM 4403 N ALA L 69	-3.288	9.568	91.926	1.00	17.58	N
	ATOM 4404 CA ALA L 69	-3.856	10.454	90.917	1.00	16.74	C
	ATOM 4405 C ALA L 69	-4.374	11.810	91.415	1.00	17.31	C
	ATOM 4406 O ALA L 69	-5.245	12.418	90.781	1.00	17.05	O
	ATOM 4407 CB ALA L 69	-4.944	9.718	90.170	1.00	16.96	C
	ATOM 4408 N GLU L 70	-3.834	12.283	92.535	1.00	17.00	N
	ATOM 4409 CA GLU L 70	-4.217	13.573	93.116	1.00	18.39	C
	ATOM 4410 C GLU L 70	-3.002	14.128	93.853	1.00	17.66	C
	ATOM 4411 O GLU L 70	-2.471	13.487	94.763	1.00	17.23	O
	ATOM 4412 CB GLU L 70	-5.395	13.410	94.090	1.00	20.10	C
	ATOM 4413 CG GLU L 70	-5.791	14.683	94.865	1.00	22.93	C
	ATOM 4414 CD GLU L 70	-6.442	15.770	93.999	1.00	23.97	C
	ATOM 4415 OE1 GLU L 70	-7.684	15.726	93.823	1.00	22.90	O
	ATOM 4416 OE2 GLU L 70	-5.721	16.683	93.521	1.00	21.68	O
	ATOM 4417 N PHE L 71	-2.541	15.299	93.436	1.00	17.15	N
	ATOM 4418 CA PHE L 71	-1.372	15.917	94.049	1.00	16.67	C
	ATOM 4419 C PHE L 71	-1.693	17.361	94.447	1.00	15.90	C
	ATOM 4420 O PHE L 71	-2.726	17.903	94.055	1.00	13.13	O
	ATOM 4421 CB PHE L 71	-0.179	15.873	93.079	1.00	17.73	C
	ATOM 4422 CG PHE L 71	0.061	14.512	92.449	1.00	17.75	C
	ATOM 4423 CD1 PHE L 71	-0.617	14.132	91.297	1.00	18.46	C
	ATOM 4424 CD2 PHE L 71	1.000	13.635	92.980	1.00	18.02	C
	ATOM 4425 CE1 PHE L 71	-0.350	12.895	90.683	1.00	18.94	C
	ATOM 4426 CE2 PHE L 71	1.269	12.400	92.374	1.00	15.52	C
	ATOM 4427 CZ PHE L 71	0.594	12.035	91.225	1.00	15.95	C
	ATOM 4428 N THR L 72	-0.826	17.965	95.256	1.00	17.14	N
	ATOM 4429 CA THR L 72	-1.038	19.338	95.716	1.00	18.59	C
	ATOM 4430 C THR L 72	0.308	20.030	95.850	1.00	18.60	C
	ATOM 4431 O THR L 72	1.330	19.384	96.096	1.00	19.31	O
	ATOM 4432 CB THR L 72	-1.731	19.401	97.105	1.00	19.45	C
	ATOM 4433 OG1 THR L 72	-2.449	18.191	97.362	1.00	23.15	O
	ATOM 4434 CG2 THR L 72	-2.728	20.537	97.143	1.00	20.85	C
	ATOM 4435 N LEU L 72	0.200	21.243	95.661	1.00	19.01	N

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FIG. 53-71	ATOM 4437	C LEUL 73	1.135	23.325	96.651	1.00	18.73	C
	ATOM 4438	O LEUL 73	0.341	24.181	96.264	1.00	19.04	O
	ATOM 4439	CB LEUL 73	1.931	22.654	94.378	1.00	13.93	C
	ATOM 4440	CG LEUL 73	3.248	23.422	94.164	1.00	10.08	C
	ATOM 4441	CD1 LEUL 73	3.006	24.909	94.249	1.00	6.04	C
	ATOM 4442	CD2 LEUL 73	4.359	22.939	95.109	1.00	4.51	C
	ATOM 4443	N THRL 74	1.677	23.327	97.862	1.00	19.96	N
	ATOM 4444	CA THRL 74	1.413	24.378	98.823	1.00	21.66	C
	ATOM 4445	C THRL 74	2.544	25.416	98.853	1.00	22.64	C
	ATOM 4446	O THRL 74	3.727	25.062	98.788	1.00	24.72	O
	ATOM 4447	CB THRL 74	1.236	23.766	100.233	1.00	22.41	C
	ATOM 4448	OG1 THRL 74	0.078	22.918	100.249	1.00	21.89	O
	ATOM 4449	CG2 THRL 74	1.084	24.855	101.289	1.00	22.57	C
	ATOM 4450	N ILEL 75	2.176	26.693	98.902	1.00	21.64	N
	ATOM 4451	CA ILEL 75	3.153	27.774	98.992	1.00	22.01	C
	ATOM 4452	C ILEL 75	2.686	28.628	100.173	1.00	24.00	C
	ATOM 4453	O ILEL 75	1.806	29.480	100.022	1.00	25.32	O
	ATOM 4454	CB ILEL 75	3.182	28.662	97.737	1.00	19.75	C
	ATOM 4455	CG1 ILEL 75	3.278	27.810	96.470	1.00	18.53	C
	ATOM 4456	CG2 ILEL 75	4.372	29.614	97.814	1.00	16.78	C
	ATOM 4457	CD1 ILEL 75	3.065	28.592	95.192	1.00	14.90	C
	ATOM 4458	N SERL 76	3.237	28.365	101.353	1.00	23.50	N
	ATOM 4459	CA SERL 76	2.853	29.102	102.545	1.00	23.97	C
	ATOM 4460	C SERL 76	2.974	30.618	102.378	1.00	24.28	C
	ATOM 4461	O SERL 76	2.066	31.247	101.864	1.00	25.23	O
	ATOM 4462	CB SERL 76	3.640	28.603	103.763	1.00	24.58	C
	ATOM 4463	OG SERL 76	3.291	27.265	104.094	1.00	22.71	O
	ATOM 4464	N SERL 77	4.090	31.200	102.787	1.00	25.69	N
	ATOM 4465	CA SERL 77	4.274	32.643	102.672	1.00	26.77	C
	ATOM 4466	C SERL 77	4.487	33.075	101.225	1.00	27.16	C
	ATOM 4467	O SERL 77	5.613	33.020	100.727	1.00	28.12	O
	ATOM 4468	CB SERL 77	5.480	33.087	103.508	1.00	28.35	C
	ATOM 4469	OG SERL 77	6.670	32.393	103.132	1.00	29.03	O
	ATOM 4470	N LEUL 78	3.410	33.476	100.547	1.00	26.54	N
	ATOM 4471	CA LEUL 78	3.487	33.931	99.151	1.00	24.64	C
	ATOM 4472	C LEUL 78	4.207	35.259	99.033	1.00	24.02	C
	ATOM 4473	O LEUL 78	3.738	36.264	99.554	1.00	25.66	O
	ATOM 4474	CB LEUL 78	2.092	34.126	98.583	1.00	23.31	C
	ATOM 4475	CG LEUL 78	1.235	32.905	98.339	1.00	24.24	C
	ATOM 4476	CD1 LEUL 78	-0.206	33.342	98.363	1.00	26.17	C
	ATOM 4477	CD2 LEUL 78	1.602	32.265	97.017	1.00	23.99	C
	ATOM 4478	N GLNL 79	5.331	35.289	98.337	1.00	23.25	N
	ATOM 4479	CA GLNL 79	6.042	36.551	98.181	1.00	24.26	C
	ATOM 4480	C GLNL 79	5.583	37.170	96.869	1.00	23.90	C
	ATOM 4481	O GLNL 79	4.446	36.978	96.457	1.00	25.83	O
	ATOM 4482	CB GLNL 79	7.555	36.330	98.193	1.00	25.76	C
	ATOM 4483	CG GLNL 79	8.029	35.324	99.242	1.00	25.88	C
	ATOM 4484	CD GLNL 79	7.585	35.657	100.648	1.00	25.29	C
	ATOM 4485	OE1 GLNL 79	6.394	35.731	100.936	1.00	23.42	O
	ATOM 4486	NE2 GLNL 79	8.546	35.858	101.535	1.00	27.79	N
	ATOM 4487	N SERL 80	6.435	37.954	96.233	1.00	22.86	N
	ATOM 4488	CA SERL 80	6.065	38.564	94.962	1.00	21.59	C
	ATOM 4489	C SERL 80	6.785	37.772	93.889	1.00	19.35	C
	ATOM 4490	O SERL 80	6.310	37.630	92.755	1.00	17.56	O
	ATOM 4491	CB SERL 80	6.491	40.037	94.935	1.00	22.61	C
	ATOM 4492	OG SERL 80	5.821	40.767	95.957	1.00	25.01	O
	ATOM 4493	N GLUL 81	7.945	37.248	94.272	1.00	16.35	N
	ATOM 4494	CA GLUL 81	8.757	36.439	93.379	1.00	15.26	C
	ATOM 4495	C GLUL 81	7.963	35.202	92.932	1.00	13.47	C
	ATOM 4496	O GLUL 81	8.163	34.694	91.832	1.00	13.42	O
	ATOM 4497	CB GLUL 81	10.075	36.053	94.071	1.00	17.15	C
	ATOM 4498	CG GLUL 81	10.052	36.176	95.614	1.00	21.02	C
	ATOM 4499	CD GLUL 81	11.404	35.897	96.265	1.00	24.30	C
	ATOM 4500	OE1 GLUL 81	12.445	36.292	95.690	1.00	25.00	O
	ATOM 4501	OE2 GLUL 81	11.426	35.281	97.358	1.00	27.51	O
	ATOM 4502	N ASPL 82	7.002	34.795	93.756	1.00	11.34	N
	ATOM 4503	CA ASPL 82	6.156	33.638	93.485	1.00	10.32	C
	ATOM 4504	C ASPL 82	5.016	33.905	92.511	1.00	9.98	C
	ATOM 4505	O ASPL 82	4.026	33.171	92.514	1.00	8.00	O
	ATOM 4506	CB ASPL 82	5.557	32.000	94.786	1.00	10.76	C



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FIG. 53-72

ATOM 4508	OD1 ASPL 82	7.804	32.822	95.533	1.00	15.38	O
ATOM 4509	OD2 ASPL 82	6.201	32.798	97.037	1.00	14.01	O
ATOM 4510	N PHEL 83	5.093	35.003	91.759	1.00	10.15	N
ATOM 4511	CA PHEL 83	4.058	35.300	90.769	1.00	10.36	C
ATOM 4512	C PHEL 83	4.445	34.421	89.588	1.00	10.31	C
ATOM 4513	O PHEL 83	5.624	34.375	89.233	1.00	10.34	O
ATOM 4514	CB PHEL 83	4.088	36.785	90.348	1.00	12.04	C
ATOM 4515	CG PHEL 83	5.208	37.142	89.388	1.00	11.12	C
ATOM 4516	CD1 PHEL 83	6.455	37.556	89.865	1.00	10.48	C
ATOM 4517	CD2 PHEL 83	5.008	37.061	88.002	1.00	9.32	C
ATOM 4518	CE1 PHEL 83	7.490	37.881	88.987	1.00	7.84	C
ATOM 4519	CE2 PHEL 83	6.030	37.382	87.108	1.00	6.55	C
ATOM 4520	CZ PHEL 83	7.277	37.795	87.600	1.00	9.45	C
ATOM 4521	N ALAL 84	3.501	33.662	89.046	1.00	9.69	N
ATOM 4522	CA ALAL 84	3.775	32.800	87.893	1.00	10.39	C
ATOM 4523	C ALAL 84	2.671	31.789	87.674	1.00	10.20	C
ATOM 4524	O ALAL 84	1.648	31.799	88.384	1.00	10.33	O
ATOM 4525	CB ALAL 84	5.105	32.066	88.055	1.00	10.16	C
ATOM 4526	N VALL 85	2.866	30.973	86.638	1.00	8.46	N
ATOM 4527	CA VALL 85	1.947	29.904	86.282	1.00	7.17	C
ATOM 4528	C VALL 85	2.655	28.652	86.785	1.00	7.11	C
ATOM 4529	O VALL 85	3.887	28.567	86.706	1.00	7.67	O
ATOM 4530	CB VALL 85	1.760	29.764	84.747	1.00	6.11	C
ATOM 4531	CG1 VALL 85	0.664	28.764	84.445	1.00	7.72	C
ATOM 4532	CG2 VALL 85	1.433	31.083	84.109	1.00	2.81	C
ATOM 4533	N TYRL 86	1.891	27.696	87.304	1.00	6.77	N
ATOM 4534	CA TYRL 86	2.449	26.447	87.824	1.00	5.61	C
ATOM 4535	C TYRL 86	1.930	25.291	87.008	1.00	6.30	C
ATOM 4536	O TYRL 86	0.756	25.276	86.630	1.00	7.74	O
ATOM 4537	CB TYRL 86	2.079	26.279	89.298	1.00	5.06	C
ATOM 4538	CG TYRL 86	2.806	27.282	90.151	1.00	4.06	C
ATOM 4539	CD1 TYRL 86	2.281	28.558	90.369	1.00	4.49	C
ATOM 4540	CD2 TYRL 86	4.076	27.001	90.640	1.00	5.08	C
ATOM 4541	CE1 TYRL 86	3.015	29.532	91.046	1.00	5.20	C
ATOM 4542	CE2 TYRL 86	4.815	27.963	91.312	1.00	6.83	C
ATOM 4543	CZ TYRL 86	4.286	29.224	91.513	1.00	5.62	C
ATOM 4544	OH TYRL 86	5.033	30.169	92.170	1.00	2.98	O
ATOM 4545	N TYRL 87	2.816	24.342	86.711	1.00	6.98	N
ATOM 4546	CA TYRL 87	2.488	23.166	85.909	1.00	5.96	C
ATOM 4547	C TYRL 87	2.916	21.887	86.607	1.00	5.99	C
ATOM 4548	O TYRL 87	3.976	21.846	87.215	1.00	7.08	O
ATOM 4549	CB TYRL 87	3.250	23.209	84.584	1.00	6.25	C
ATOM 4550	CG TYRL 87	2.854	24.294	83.614	1.00	6.20	C
ATOM 4551	CD1 TYRL 87	1.660	24.218	82.902	1.00	7.29	C
ATOM 4552	CD2 TYRL 87	3.712	25.360	83.349	1.00	8.25	C
ATOM 4553	CE1 TYRL 87	1.331	25.169	81.945	1.00	7.18	C
ATOM 4554	CE2 TYRL 87	3.391	26.313	82.392	1.00	8.23	C
ATOM 4555	CZ TYRL 87	2.203	26.207	81.691	1.00	8.35	C
ATOM 4556	OH TYRL 87	1.925	27.106	80.693	1.00	12.74	O
ATOM 4557	N CYSL 88	2.139	20.824	86.442	1.00	6.86	N
ATOM 4558	CA CYSL 88	2.469	19.526	87.028	1.00	7.91	C
ATOM 4559	C CYSL 88	2.677	18.544	85.883	1.00	8.19	C
ATOM 4560	O CYSL 88	1.929	18.553	84.910	1.00	8.52	O
ATOM 4561	CB CYSL 88	1.352	19.036	87.941	1.00	8.00	C
ATOM 4562	SG CYSL 88	-0.208	18.550	87.117	1.00	14.73	S
ATOM 4563	N GLNL 89	3.698	17.704	85.988	1.00	9.10	N
ATOM 4564	CA GLNL 89	3.990	16.736	84.935	1.00	10.07	C
ATOM 4565	C GLNL 89	4.237	15.341	85.473	1.00	11.75	C
ATOM 4566	O GLNL 89	5.076	15.151	86.357	1.00	13.16	O
ATOM 4567	CB GLNL 89	5.222	17.173	84.140	1.00	7.86	C
ATOM 4568	CG GLNL 89	5.767	16.106	83.207	1.00	3.60	C
ATOM 4569	CD GLNL 89	7.268	16.200	83.025	1.00	3.91	C
ATOM 4570	OE1 GLNL 89	7.808	15.788	82.000	1.00	5.27	O
ATOM 4571	NE2 GLNL 89	7.956	16.727	84.031	1.00	2.00	N
ATOM 4572	N GLNL 90	3.529	14.364	84.919	1.00	13.92	N
ATOM 4573	CA GLNL 90	3.704	12.976	85.329	1.00	14.37	C
ATOM 4574	C GLNL 90	4.740	12.358	84.409	1.00	14.11	C
ATOM 4575	O GLNL 90	4.878	12.760	83.252	1.00	14.22	O
ATOM 4576	CB GLNL 90	2.384	12.206	85.209	1.00	16.09	C
ATOM 4577	CG GLNL 90	1.804	11.024	82.782	1.00	18.12	C

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FIG. 53-73

ATOM 4579	OE1 GLNL 90	2.745	10.772	81.861	1.00	19.12	O
ATOM 4580	NE2 GLNL 90	3.161	9.868	83.870	1.00	21.14	N
ATOM 4581	N TYRL 91	5.436	11.345	84.898	1.00	14.31	N
ATOM 4582	CA TYRL 91	6.439	10.663	84.085	1.00	14.21	C
ATOM 4583	C TYRL 91	6.583	9.230	84.563	1.00	12.81	C
ATOM 4584	O TYRL 91	7.680	8.684	84.595	1.00	12.62	O
ATOM 4585	CB TYRL 91	7.792	11.404	84.117	1.00	14.56	C
ATOM 4586	CG TYRL 91	8.262	11.779	85.501	1.00	14.78	C
ATOM 4587	CD1 TYRL 91	7.777	12.926	86.132	1.00	15.04	C
ATOM 4588	CD2 TYRL 91	9.138	10.963	86.206	1.00	14.16	C
ATOM 4589	CE1 TYRL 91	8.125	13.232	87.427	1.00	13.42	C
ATOM 4590	CE2 TYRL 91	9.495	11.266	87.517	1.00	15.16	C
ATOM 4591	CZ TYRL 91	8.981	12.405	88.117	1.00	14.10	C
ATOM 4592	OH TYRL 91	9.275	12.701	89.421	1.00	12.42	O
ATOM 4593	N ASN1 92	5.456	8.631	84.921	1.00	12.06	N
ATOM 4594	CA ASN1 92	5.441	7.259	85.409	1.00	13.38	C
ATOM 4595	C ASN1 92	5.662	6.243	84.302	1.00	13.10	C
ATOM 4596	O ASN1 92	6.606	5.453	84.364	1.00	14.86	O
ATOM 4597	CB ASN1 92	4.124	6.962	86.123	1.00	13.96	C
ATOM 4598	CG ASN1 92	4.114	5.591	86.781	1.00	16.48	C
ATOM 4599	OD1 ASN1 92	3.139	4.846	86.671	1.00	17.04	O
ATOM 4600	ND2 ASN1 92	5.188	5.264	87.489	1.00	18.14	N
ATOM 4601	N ASN1 93	4.805	6.305	83.280	1.00	11.53	N
ATOM 4602	CA ASN1 93	4.833	5.404	82.125	1.00	8.54	C
ATOM 4603	C ASN1 93	6.136	5.120	81.379	1.00	7.78	C
ATOM 4604	O ASN1 93	7.072	5.911	81.387	1.00	6.63	O
ATOM 4605	CB ASN1 93	3.749	5.798	81.110	1.00	7.89	C
ATOM 4606	CG ASN1 93	3.803	7.271	80.699	1.00	6.74	C
ATOM 4607	OD1 ASN1 93	2.901	7.754	80.029	1.00	8.49	O
ATOM 4608	ND2 ASN1 93	4.861	7.973	81.072	1.00	6.95	N
ATOM 4609	N TRPL 94	6.180	3.943	80.765	1.00	8.55	N
ATOM 4610	CA TRPL 94	7.319	3.495	79.973	1.00	8.39	C
ATOM 4611	C TRPL 94	6.777	2.509	78.928	1.00	10.86	C
ATOM 4612	O TRPL 94	6.035	1.585	79.276	1.00	13.10	O
ATOM 4613	CB TRPL 94	8.381	2.829	80.834	1.00	4.60	C
ATOM 4614	CG TRPL 94	9.621	2.575	80.051	1.00	5.78	C
ATOM 4615	CD1 TRPL 94	9.845	1.543	79.189	1.00	5.72	C
ATOM 4616	CD2 TRPL 94	10.754	3.450	79.929	1.00	6.84	C
ATOM 4617	NE1 TRPL 94	11.032	1.729	78.523	1.00	6.91	N
ATOM 4618	CE2 TRPL 94	11.610	2.893	78.956	1.00	7.01	C
ATOM 4619	CE3 TRPL 94	11.118	4.660	80.534	1.00	8.34	C
ATOM 4620	CZ2 TRPL 94	12.808	3.502	78.572	1.00	6.29	C
ATOM 4621	CZ3 TRPL 94	12.309	5.268	80.150	1.00	10.04	C
ATOM 4622	CH2 TRPL 94	13.138	4.684	79.175	1.00	8.04	C
ATOM 4623	N PROL 95	7.102	2.711	77.631	1.00	12.64	N
ATOM 4624	CA PROL 95	7.906	3.796	77.035	1.00	12.43	C
ATOM 4625	C PROL 95	7.390	5.174	77.417	1.00	11.48	C
ATOM 4626	O PROL 95	6.185	5.353	77.619	1.00	13.24	O
ATOM 4627	CB PROL 95	7.759	3.554	75.533	1.00	10.88	C
ATOM 4628	CG PROL 95	7.546	2.072	75.450	1.00	12.47	C
ATOM 4629	CD PROL 95	6.586	1.813	76.581	1.00	10.61	C
ATOM 4630	N PROL 96	8.293	6.156	77.528	1.00	10.03	N
ATOM 4631	CA PROL 96	7.989	7.541	77.888	1.00	8.83	C
ATOM 4632	C PROL 96	6.846	8.185	77.108	1.00	9.51	C
ATOM 4633	O PROL 96	6.860	8.267	75.887	1.00	9.25	O
ATOM 4634	CB PROL 96	9.308	8.251	77.614	1.00	7.78	C
ATOM 4635	CG PROL 96	10.307	7.225	77.935	1.00	8.31	C
ATOM 4636	CD PROL 96	9.735	5.995	77.277	1.00	9.84	C
ATOM 4637	N ARGL 97	5.831	8.609	77.840	1.00	11.51	N
ATOM 4638	CA ARGL 97	4.683	9.289	77.278	1.00	12.61	C
ATOM 4639	C ARGL 97	4.309	10.253	78.397	1.00	12.40	C
ATOM 4640	O ARGL 97	3.150	10.333	78.823	1.00	12.94	O
ATOM 4641	CB ARGL 97	3.556	8.302	77.017	1.00	17.09	C
ATOM 4642	CG ARGL 97	3.857	7.269	75.947	1.00	22.39	C
ATOM 4643	CD ARGL 97	2.971	6.037	76.132	1.00	26.24	C
ATOM 4644	NE ARGL 97	3.286	5.283	77.346	1.00	28.09	N
ATOM 4645	CZ ARGL 97	3.788	4.054	77.352	1.00	28.60	C
ATOM 4646	NH1 ARGL 97	4.040	3.434	76.209	1.00	30.10	N
ATOM 4647	NH2 ARGL 97	4.023	3.439	78.499	1.00	29.71	N
ATOM 4648	N TYR1 98	5.245	10.018	78.012	1.00	11.60	N

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FIG. 53-74

ATOM 4650 C TYR L 98	4.363	13.058	79.558	1.00	11.64	C
ATOM 4651 O TYR L 98	4.478	13.527	78.421	1.00	13.48	O
ATOM 4652 CB TYR L 98	6.636	12.364	80.400	1.00	12.53	C
ATOM 4653 CG TYR L 98	7.664	11.252	80.600	1.00	13.17	C
ATOM 4654 CD1 TYR L 98	7.276	9.916	80.785	1.00	10.99	C
ATOM 4655 CD2 TYR L 98	9.035	11.543	80.599	1.00	14.00	C
ATOM 4656 CE1 TYR L 98	8.229	8.897	80.961	1.00	9.87	C
ATOM 4657 CE2 TYR L 98	9.993	10.534	80.780	1.00	14.26	C
ATOM 4658 CZ TYR L 98	9.582	9.212	80.958	1.00	13.39	C
ATOM 4659 OH TYR L 98	10.531	8.229	81.125	1.00	8.87	O
ATOM 4660 N THR L 99	3.493	13.536	80.439	1.00	9.53	N
ATOM 4661 CA THR L 99	2.573	14.609	80.067	1.00	9.79	C
ATOM 4662 C THR L 99	2.517	15.767	81.051	1.00	9.59	C
ATOM 4663 O THR L 99	2.939	15.640	82.198	1.00	9.97	O
ATOM 4664 CB THR L 99	1.127	14.042	79.884	1.00	12.13	C
ATOM 4665 OG1 THR L 99	0.721	13.338	81.072	1.00	10.31	O
ATOM 4666 CG2 THR L 99	1.065	13.079	78.692	1.00	11.41	C
ATOM 4667 N PHE L 100	1.964	16.889	80.601	1.00	10.05	N
ATOM 4668 CA PHE L 100	1.822	18.087	81.430	1.00	7.56	C
ATOM 4669 C PHE L 100	0.360	18.422	81.683	1.00	8.42	C
ATOM 4670 O PHE L 100	-0.547	17.900	81.012	1.00	6.96	O
ATOM 4671 CB PHE L 100	2.443	19.297	80.738	1.00	4.66	C
ATOM 4672 CG PHE L 100	3.932	19.339	80.795	1.00	3.07	C
ATOM 4673 CD1 PHE L 100	4.694	18.736	79.812	1.00	5.57	C
ATOM 4674 CD2 PHE L 100	4.575	20.000	81.827	1.00	2.00	C
ATOM 4675 CE1 PHE L 100	6.090	18.792	79.857	1.00	6.31	C
ATOM 4676 CE2 PHE L 100	5.955	20.062	81.884	1.00	2.00	C
ATOM 4677 CZ PHE L 100	6.718	19.458	80.899	1.00	3.05	C
ATOM 4678 N GLY L 101	0.144	19.279	82.673	1.00	9.22	N
ATOM 4679 CA GLY L 101	-1.191	19.749	82.987	1.00	10.55	C
ATOM 4680 C GLY L 101	-1.278	21.122	82.336	1.00	11.54	C
ATOM 4681 O GLY L 101	-0.242	21.720	82.025	1.00	10.78	O
ATOM 4682 N GLN L 102	-2.490	21.640	82.145	1.00	13.06	N
ATOM 4683 CA GLN L 102	-2.669	22.948	81.515	1.00	13.20	C
ATOM 4684 C GLN L 102	-2.292	24.155	82.397	1.00	12.85	C
ATOM 4685 O GLN L 102	-2.497	25.310	82.011	1.00	12.27	O
ATOM 4686 CB GLN L 102	-4.095	23.093	80.972	1.00	14.24	C
ATOM 4687 CG GLN L 102	-5.117	23.675	81.947	1.00	15.34	C
ATOM 4688 CD GLN L 102	-5.437	22.758	83.107	1.00	16.33	C
ATOM 4689 OE1 GLN L 102	-4.986	21.602	83.155	1.00	14.14	O
ATOM 4690 NE2 GLN L 102	-6.206	23.275	84.069	1.00	14.33	N
ATOM 4691 N GLY L 103	-1.759	23.882	83.582	1.00	12.36	N
ATOM 4692 CA GLY L 103	-1.343	24.946	84.475	1.00	12.60	C
ATOM 4693 C GLY L 103	-2.389	25.690	85.285	1.00	12.40	C
ATOM 4694 O GLY L 103	-3.561	25.765	84.909	1.00	13.24	O
ATOM 4695 N THR L 104	-1.938	26.228	86.414	1.00	11.51	N
ATOM 4696 CA THR L 104	-2.757	27.013	87.330	1.00	11.59	C
ATOM 4697 C THR L 104	-2.092	28.388	87.324	1.00	10.45	C
ATOM 4698 O THR L 104	-0.864	28.466	87.408	1.00	10.03	O
ATOM 4699 CB THR L 104	-2.712	26.423	88.767	1.00	13.28	C
ATOM 4700 OG1 THR L 104	-3.350	25.137	88.778	1.00	16.79	O
ATOM 4701 CG2 THR L 104	-3.419	27.338	89.769	1.00	13.46	C
ATOM 4702 N ARG L 105	-2.875	29.449	87.112	1.00	9.53	N
ATOM 4703 CA ARG L 105	-2.347	30.816	87.092	1.00	10.17	C
ATOM 4704 C ARG L 105	-2.426	31.411	88.487	1.00	8.72	C
ATOM 4705 O ARG L 105	-3.518	31.591	89.019	1.00	6.15	O
ATOM 4706 CB ARG L 105	-3.155	31.694	86.139	1.00	13.45	C
ATOM 4707 CG ARG L 105	-2.867	31.481	84.655	1.00	18.32	C
ATOM 4708 CD ARG L 105	-4.156	31.289	83.851	1.00	18.07	C
ATOM 4709 NE ARG L 105	-4.578	29.894	83.843	1.00	16.55	N
ATOM 4710 CZ ARG L 105	-4.026	28.966	83.071	1.00	21.31	C
ATOM 4711 NH1 ARG L 105	-3.029	29.295	82.247	1.00	21.54	N
ATOM 4712 NH2 ARG L 105	-4.455	27.707	83.127	1.00	24.25	N
ATOM 4713 N LEU L 106	-1.277	31.728	89.074	1.00	9.90	N
ATOM 4714 CA LEU L 106	-1.245	32.285	90.426	1.00	12.46	C
ATOM 4715 C LEU L 106	-1.020	33.805	90.440	1.00	12.71	C
ATOM 4716 O LEU L 106	0.115	34.271	90.356	1.00	12.95	O
ATOM 4717 CB LEU L 106	-0.172	31.576	91.260	1.00	12.39	C
ATOM 4718 CG LEU L 106	-0.065	32.022	92.726	1.00	13.06	C
ATOM 4719 CD LEU L 106	-1.407	31.857	89.417	1.00	9.05	C

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FIG. 53-75

ATOM 4721 N GLUL 107	-2.101 34.565 90.582 1.00 13.08	N
ATOM 4722 CA GLUL 107	-2.013 36.017 90.589 1.00 14.42	C
ATOM 4723 C GLUL 107	-2.267 36.679 91.951 1.00 15.47	C
ATOM 4724 O GLUL 107	-2.788 36.054 92.893 1.00 14.67	O
ATOM 4725 CB GLUL 107	-2.953 36.600 89.543 1.00 14.27	C
ATOM 4726 CG GLUL 107	-4.399 36.226 89.770 1.00 14.41	C
ATOM 4727 CD GLUL 107	-5.297 37.432 89.928 1.00 14.83	C
ATOM 4728 OE1 GLUL 107	-5.148 38.404 89.161 1.00 15.25	O
ATOM 4729 OE2 GLUL 107	-6.162 37.405 90.822 1.00 14.96	O
ATOM 4730 N ILEL 108	-1.897 37.961 92.021 1.00 15.44	N
ATOM 4731 CA ILEL 108	-2.022 38.796 93.217 1.00 12.47	C
ATOM 4732 C ILEL 108	-3.435 39.342 93.374 1.00 12.47	C
ATOM 4733 O ILEL 108	-3.965 39.993 92.468 1.00 11.83	O
ATOM 4734 CB ILEL 108	-1.067 40.007 93.148 1.00 11.33	C
ATOM 4735 CG1 ILEL 108	0.359 39.544 92.842 1.00 8.42	C
ATOM 4736 CG2 ILEL 108	-1.130 40.784 94.447 1.00 11.29	C
ATOM 4737 CD1 ILEL 108	1.342 40.645 92.658 1.00 8.08	C
ATOM 4738 N LYSL 109	-4.040 39.079 94.528 1.00 12.15	N
ATOM 4739 CA LYSL 109	-5.384 39.555 94.803 1.00 12.07	C
ATOM 4740 C LYSL 109	-5.281 40.868 95.566 1.00 13.37	C
ATOM 4741 O LYSL 109	-4.522 40.976 96.531 1.00 14.27	O
ATOM 4742 CB LYSL 109	-6.168 38.539 95.634 1.00 10.80	C
ATOM 4743 CG LYSL 109	-7.660 38.849 95.710 1.00 10.92	C
ATOM 4744 CD LYSL 109	-8.262 38.428 97.030 1.00 11.47	C
ATOM 4745 CE LYSL 109	-8.214 36.937 97.205 1.00 14.99	C
ATOM 4746 NZ LYSL 109	-8.792 36.548 98.511 1.00 17.24	N
ATOM 4747 N ARGL 110	-6.031 41.866 95.124 1.00 13.56	N
ATOM 4748 CA ARGL 110	-6.031 43.169 95.768 1.00 13.88	C
ATOM 4749 C ARGL 110	-7.455 43.693 95.698 1.00 14.01	C
ATOM 4750 O ARGL 110	-8.385 42.927 95.436 1.00 14.87	O
ATOM 4751 CB ARGL 110	-5.078 44.124 95.048 1.00 14.70	C
ATOM 4752 CG ARGL 110	-5.293 44.201 93.553 1.00 17.17	C
ATOM 4753 CD ARGL 110	-4.842 45.537 92.996 1.00 20.25	C
ATOM 4754 NE ARGL 110	-5.734 46.629 93.378 1.00 22.67	N
ATOM 4755 CZ ARGL 110	-5.412 47.919 93.308 1.00 24.63	C
ATOM 4756 NH1 ARGL 110	-4.211 48.294 92.872 1.00 25.47	N
ATOM 4757 NH2 ARGL 110	-6.296 48.839 93.676 1.00 24.14	N
ATOM 4758 N THRL 111	-7.642 44.979 95.961 1.00 13.27	N
ATOM 4759 CA THRL 111	-8.980 45.552 95.901 1.00 12.64	C
ATOM 4760 C THRL 111	-9.415 45.912 94.480 1.00 12.65	C
ATOM 4761 O THRL 111	-8.590 46.132 93.581 1.00 12.06	O
ATOM 4762 CB THRL 111	-9.134 46.786 96.830 1.00 10.77	C
ATOM 4763 OG1 THRL 111	-7.977 47.627 96.726 1.00 9.50	O
ATOM 4764 CG2 THRL 111	-9.312 46.340 98.269 1.00 11.72	C
ATOM 4765 N VALL 112	-10.726 45.947 94.291 1.00 12.84	N
ATOM 4766 CA VALL 112	-11.322 46.282 93.018 1.00 14.13	C
ATOM 4767 C VALL 112	-11.036 47.735 92.676 1.00 14.88	C
ATOM 4768 O VALL 112	-11.193 48.634 93.508 1.00 17.13	O
ATOM 4769 CB VALL 112	-12.844 46.059 93.066 1.00 15.42	C
ATOM 4770 CG1 VALL 112	-13.497 46.510 91.765 1.00 13.79	C
ATOM 4771 CG2 VALL 112	-13.140 44.590 93.360 1.00 14.81	C
ATOM 4772 N ALAL 113	-10.612 47.946 91.443 1.00 14.08	N
ATOM 4773 CA ALAL 113	-10.290 49.263 90.930 1.00 11.78	C
ATOM 4774 C ALAL 113	-10.817 49.317 89.504 1.00 11.36	C
ATOM 4775 O ALAL 113	-10.383 48.544 88.649 1.00 11.74	O
ATOM 4776 CB ALAL 113	-8.774 49.462 90.938 1.00 9.94	C
ATOM 4777 N ALAL 114	-11.789 50.188 89.263 1.00 11.49	N
ATOM 4778 CA ALAL 114	-12.382 50.349 87.931 1.00 10.65	C
ATOM 4779 C ALAL 114	-11.345 50.830 86.924 1.00 10.71	C
ATOM 4780 O ALAL 114	-10.319 51.378 87.309 1.00 10.78	O
ATOM 4781 CB ALAL 114	-13.543 51.330 87.990 1.00 8.85	C
ATOM 4782 N PROL 115	-11.567 50.556 85.624 1.00 12.64	N
ATOM 4783 CA PROL 115	-10.646 50.971 84.558 1.00 13.53	C
ATOM 4784 C PROL 115	-10.870 52.386 84.047 1.00 14.19	C
ATOM 4785 O PROL 115	-12.002 52.846 83.938 1.00 15.12	O
ATOM 4786 CB PROL 115	-10.921 49.949 83.456 1.00 14.01	C
ATOM 4787 CG PROL 115	-12.370 49.662 83.627 1.00 13.50	C
ATOM 4788 CD PROL 115	-12.509 49.537 85.123 1.00 12.92	C
ATOM 4789 N SERL 116	-9.779 53.080 83.751 1.00 15.47	N
ATOM 4790 CA SERL 116	-9.847 54.420 83.214 1.00 15.68	C

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FIG. 53-76

ATOM 4792 O SER L 116	-8.903	53.937	81.078	1.00	18.27	O
ATOM 4793 CB SER L 116	-8.580	55.212	83.568	1.00	15.35	C
ATOM 4794 OG SER L 116	-8.371	55.226	84.972	1.00	15.79	O
ATOM 4795 N VAL L 117	-11.136	54.218	81.181	1.00	16.94	N
ATOM 4796 CA VAL L 117	-11.356	53.979	79.755	1.00	16.67	C
ATOM 4797 C VAL L 117	-10.901	55.136	78.862	1.00	17.18	C
ATOM 4798 O VAL L 117	-10.979	56.307	79.250	1.00	18.64	O
ATOM 4799 CB VAL L 117	-12.840	53.652	79.481	1.00	16.30	C
ATOM 4800 CG1 VAL L 117	-13.031	53.215	78.038	1.00	17.39	C
ATOM 4801 CG2 VAL L 117	-13.317	52.565	80.439	1.00	12.57	C
ATOM 4802 N PHE L 118	-10.394	54.803	77.680	1.00	16.97	N
ATOM 4803 CA PHE L 118	-9.928	55.800	76.720	1.00	16.16	C
ATOM 4804 C PHE L 118	-10.135	55.272	75.305	1.00	16.79	C
ATOM 4805 O PHE L 118	-9.853	54.112	75.030	1.00	17.04	O
ATOM 4806 CB PHE L 118	-8.444	56.094	76.928	1.00	15.58	C
ATOM 4807 CG PHE L 118	-8.118	56.652	78.279	1.00	16.00	C
ATOM 4808 CD1 PHE L 118	-8.615	57.892	78.675	1.00	16.23	C
ATOM 4809 CD2 PHE L 118	-7.316	55.933	79.163	1.00	14.89	C
ATOM 4810 CE1 PHE L 118	-8.323	58.409	79.933	1.00	14.96	C
ATOM 4811 CE2 PHE L 118	-7.016	56.438	80.420	1.00	14.32	C
ATOM 4812 CZ PHE L 118	-7.521	57.682	80.808	1.00	16.00	C
ATOM 4813 N ILE L 119	-10.640	56.117	74.412	1.00	16.97	N
ATOM 4814 CA ILE L 119	-10.867	55.710	73.033	1.00	18.14	C
ATOM 4815 C ILE L 119	-9.896	56.477	72.135	1.00	18.40	C
ATOM 4816 O ILE L 119	-9.322	57.490	72.558	1.00	18.80	O
ATOM 4817 CB ILE L 119	-12.340	55.958	72.594	1.00	17.61	C
ATOM 4818 CG1 ILE L 119	-12.703	55.036	71.430	1.00	15.98	C
ATOM 4819 CG2 ILE L 119	-12.550	57.413	72.181	1.00	19.09	C
ATOM 4820 CD1 ILE L 119	-14.149	55.164	70.973	1.00	16.09	C
ATOM 4821 N PHE L 120	-9.677	55.961	70.928	1.00	18.54	N
ATOM 4822 CA PHE L 120	-8.773	56.576	69.957	1.00	19.20	C
ATOM 4823 C PHE L 120	-9.305	56.406	68.533	1.00	19.76	C
ATOM 4824 O PHE L 120	-9.706	55.312	68.149	1.00	21.23	O
ATOM 4825 CB PHE L 120	-7.378	55.939	70.023	1.00	16.85	C
ATOM 4826 CG PHE L 120	-6.653	56.159	71.324	1.00	16.80	C
ATOM 4827 CD1 PHE L 120	-6.334	57.450	71.756	1.00	15.81	C
ATOM 4828 CD2 PHE L 120	-6.226	55.069	72.092	1.00	15.45	C
ATOM 4829 CE1 PHE L 120	-5.592	57.652	72.937	1.00	15.59	C
ATOM 4830 CE2 PHE L 120	-5.486	55.259	73.274	1.00	15.71	C
ATOM 4831 CZ PHE L 120	-5.167	56.549	73.696	1.00	14.12	C
ATOM 4832 N PRO L 121	-9.424	57.509	67.779	1.00	20.16	N
ATOM 4833 CA PRO L 121	-9.912	57.430	66.401	1.00	21.06	C
ATOM 4834 C PRO L 121	-8.778	56.938	65.504	1.00	20.94	C
ATOM 4835 O PRO L 121	-7.620	56.947	65.913	1.00	20.50	O
ATOM 4836 CB PRO L 121	-10.257	58.890	66.082	1.00	21.51	C
ATOM 4837 CG PRO L 121	-10.567	59.482	67.416	1.00	21.20	C
ATOM 4838 CD PRO L 121	-9.470	58.901	68.262	1.00	20.05	C
ATOM 4839 N PRO L 122	-9.098	56.463	64.287	1.00	22.00	N
ATOM 4840 CA PRO L 122	-8.067	55.978	63.360	1.00	22.92	C
ATOM 4841 C PRO L 122	-7.288	57.181	62.836	1.00	23.88	C
ATOM 4842 O PRO L 122	-7.871	58.112	62.285	1.00	24.51	O
ATOM 4843 CB PRO L 122	-8.885	55.337	62.235	1.00	22.26	C
ATOM 4844 CG PRO L 122	-10.181	54.978	62.887	1.00	22.25	C
ATOM 4845 CD PRO L 122	-10.441	56.183	63.759	1.00	22.67	C
ATOM 4846 N SER L 123	-5.973	57.158	63.005	1.00	25.66	N
ATOM 4847 CA SER L 123	-5.112	58.252	62.571	1.00	26.94	C
ATOM 4848 C SER L 123	-5.327	58.635	61.115	1.00	28.60	C
ATOM 4849 O SER L 123	-5.534	57.773	60.259	1.00	28.79	O
ATOM 4850 CB SER L 123	-3.648	57.859	62.765	1.00	27.37	C
ATOM 4851 OG SER L 123	-3.335	56.701	62.003	1.00	24.63	O
ATOM 4852 N ASP L 124	-5.222	59.927	60.829	1.00	30.29	N
ATOM 4853 CA ASP L 124	-5.381	60.419	59.467	1.00	31.10	C
ATOM 4854 C ASP L 124	-4.416	59.704	58.549	1.00	31.06	C
ATOM 4855 O ASP L 124	-4.741	59.436	57.395	1.00	31.07	O
ATOM 4856 CB ASP L 124	-5.141	61.927	59.396	1.00	32.87	C
ATOM 4857 CG ASP L 124	-6.390	62.726	59.691	1.00	34.61	C
ATOM 4858 OD1 ASP L 124	-7.349	62.599	58.902	1.00	34.85	O
ATOM 4859 OD2 ASP L 124	-6.411	63.472	60.694	1.00	34.61	O
ATOM 4860 N GLU L 125	-3.232	59.404	59.073	1.00	30.87	N
ATOM 4861 CA GLU L 125	-2.108	58.607	58.337	1.00	31.80	C

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FIG. 53-77	ATOM 4863 O GLUL 125	-2.379	56.786	56.868	1.00	32.57	O
	ATOM 4864 CB GLUL 125	-0.927	58.622	59.182	1.00	31.97	C
	ATOM 4865 CG GLUL 125	0.150	57.698	58.639	1.00	34.49	C
	ATOM 4866 CD GLUL 125	1.429	57.742	59.454	1.00	35.13	C
	ATOM 4867 OE1 GLUL 125	1.416	58.245	60.604	1.00	35.50	O
	ATOM 4868 OE2 GLUL 125	2.465	57.269	58.940	1.00	35.88	O
	ATOM 4869 N GLNL 126	-3.412	56.638	58.865	1.00	32.79	N
	ATOM 4870 CA GLNL 126	-3.931	55.304	58.603	1.00	32.46	C
	ATOM 4871 C GLNL 126	-5.097	55.409	57.619	1.00	33.57	C
	ATOM 4872 O GLNL 126	-5.278	54.550	56.749	1.00	34.07	O
	ATOM 4873 CB GLNL 126	-4.392	54.624	59.887	1.00	30.48	C
	ATOM 4874 CG GLNL 126	-4.513	53.127	59.743	1.00	27.57	C
	ATOM 4875 CD GLNL 126	-5.088	52.462	60.963	1.00	27.43	C
	ATOM 4876 OE1 GLNL 126	-6.161	52.828	61.438	1.00	25.65	O
	ATOM 4877 NE2 GLNL 126	-4.384	51.465	61.477	1.00	27.30	N
	ATOM 4878 N LEUL 127	-5.879	56.473	57.748	1.00	34.76	N
	ATOM 4879 CA LEUL 127	-7.001	56.700	56.848	1.00	36.08	C
	ATOM 4880 C LEUL 127	-6.476	56.986	55.436	1.00	37.31	C
	ATOM 4881 O LEUL 127	-7.070	56.554	54.442	1.00	36.78	O
	ATOM 4882 CB LEUL 127	-7.859	57.870	57.345	1.00	36.18	C
	ATOM 4883 CG LEUL 127	-9.224	57.533	57.961	1.00	36.61	C
	ATOM 4884 CD1 LEUL 127	-9.050	56.630	59.160	1.00	37.63	C
	ATOM 4885 CD2 LEUL 127	-9.963	58.812	58.348	1.00	35.88	C
	ATOM 4886 N LYSL 128	-5.377	57.729	55.342	1.00	38.69	N
	ATOM 4887 CA LYSL 128	-4.799	58.038	54.037	1.00	40.81	C
	ATOM 4888 C LYSL 128	-4.191	56.746	53.497	1.00	41.40	C
	ATOM 4889 O LYSL 128	-4.427	56.377	52.343	1.00	42.64	O
	ATOM 4890 CB LYSL 128	-3.703	59.118	54.126	1.00	42.31	C
	ATOM 4891 CG LYSL 128	-4.062	60.396	54.884	1.00	42.79	C
	ATOM 4892 CD LYSL 128	-5.250	61.141	54.301	1.00	43.43	C
	ATOM 4893 CE LYSL 128	-5.690	62.278	55.228	1.00	43.12	C
	ATOM 4894 NZ LYSL 128	-6.313	61.792	56.503	1.00	41.82	N
	ATOM 4895 N SERL 129	-3.459	56.037	54.361	1.00	40.89	N
	ATOM 4896 CA SERL 129	-2.805	54.788	53.980	1.00	39.68	C
	ATOM 4897 C SERL 129	-3.800	53.757	53.462	1.00	38.38	C
	ATOM 4898 O SERL 129	-3.427	52.894	52.668	1.00	38.82	O
	ATOM 4899 CB SERL 129	-1.978	54.210	55.137	1.00	40.35	C
	ATOM 4900 OG SERL 129	-2.786	53.539	56.090	1.00	41.44	O
	ATOM 4901 N GLYL 130	-5.044	53.816	53.943	1.00	36.60	N
	ATOM 4902 CA GLYL 130	-6.058	52.894	53.455	1.00	34.28	C
	ATOM 4903 C GLYL 130	-6.965	52.141	54.415	1.00	33.04	C
	ATOM 4904 O GLYL 130	-7.991	51.603	53.983	1.00	32.64	O
	ATOM 4905 N THRL 131	-6.631	52.100	55.700	1.00	31.29	N
	ATOM 4906 CA THRL 131	-7.456	51.366	56.658	1.00	29.86	C
	ATOM 4907 C THRL 131	-7.819	52.215	57.876	1.00	28.24	C
	ATOM 4908 O THRL 131	-7.146	53.199	58.177	1.00	28.47	O
	ATOM 4909 CB THRL 131	-6.749	50.056	57.102	1.00	30.36	C
	ATOM 4910 OG1 THRL 131	-6.373	49.301	55.944	1.00	32.17	O
	ATOM 4911 CG2 THRL 131	-7.670	49.191	57.942	1.00	31.50	C
	ATOM 4912 N ALAL 132	-8.915	51.852	58.542	1.00	26.77	N
	ATOM 4913 CA ALAL 132	-9.389	52.560	59.728	1.00	24.76	C
	ATOM 4914 C ALAL 132	-9.377	51.630	60.943	1.00	22.96	C
	ATOM 4915 O ALAL 132	-10.031	50.586	60.937	1.00	22.49	O
	ATOM 4916 CB ALAL 132	-10.789	53.079	59.484	1.00	26.60	C
	ATOM 4917 N SERL 133	-8.630	52.007	61.976	1.00	21.32	N
	ATOM 4918 CA SERL 133	-8.522	51.200	63.187	1.00	19.59	C
	ATOM 4919 C SERL 133	-8.748	52.028	64.444	1.00	18.17	C
	ATOM 4920 O SERL 133	-7.912	52.856	64.819	1.00	17.68	O
	ATOM 4921 CB SERL 133	-7.148	50.532	63.253	1.00	20.02	C
	ATOM 4922 OG SERL 133	-6.865	49.830	62.053	1.00	20.61	O
	ATOM 4923 N VALL 134	-9.901	51.824	65.070	1.00	16.47	N
	ATOM 4924 CA VALL 134	-10.254	52.549	66.279	1.00	15.50	C
	ATOM 4925 C VALL 134	-9.679	51.711	67.417	1.00	15.65	C
	ATOM 4926 O VALL 134	-9.483	50.498	67.257	1.00	17.17	O
	ATOM 4927 CB VALL 134	-11.800	52.697	66.415	1.00	15.27	C
	ATOM 4928 CG1 VALL 134	-12.149	53.794	67.418	1.00	11.88	C
	ATOM 4929 CG2 VALL 134	-12.423	52.997	65.065	1.00	11.45	C
	ATOM 4930 N VALL 135	-9.383	52.343	68.548	1.00	13.24	N
	ATOM 4931 CA VALL 135	-8.792	51.633	69.668	1.00	11.67	C
	ATOM 4932 C VALL 135	-8.208	52.078	70.084	1.00	12.50	C

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FIG. 53-78	ATOM 4934	CB VALL 135	-7.258	51.890	69.734	1.00	9.22	C
	ATOM 4935	CG1 VALL 135	-6.637	51.171	70.913	1.00	7.65	C
	ATOM 4936	CG2 VALL 135	-6.594	51.457	68.457	1.00	6.97	C
	ATOM 4937	N CYSL 136	-9.693	51.127	71.861	1.00	11.53	N
	ATOM 4938	CA CYSL 136	-10.219	51.471	73.165	1.00	11.78	C
	ATOM 4939	C CYSL 136	-9.256	50.871	74.173	1.00	11.17	C
	ATOM 4940	O CYSL 136	-8.738	49.769	73.957	1.00	10.47	O
	ATOM 4941	CB CYSL 136	-11.619	50.925	73.374	1.00	13.27	C
	ATOM 4942	SG CYSL 136	-12.448	51.737	74.772	1.00	16.80	S
	ATOM 4943	N LEUL 137	-9.046	51.592	75.273	1.00	9.86	N
	ATOM 4944	CA LEUL 137	-8.109	51.210	76.316	1.00	8.87	C
	ATOM 4945	C LEUL 137	-8.717	51.281	77.712	1.00	9.05	C
	ATOM 4946	O LEUL 137	-9.136	52.350	78.173	1.00	9.00	O
	ATOM 4947	CB LEUL 137	-6.911	52.167	76.258	1.00	8.33	C
	ATOM 4948	CG LEUL 137	-5.549	51.962	76.945	1.00	9.11	C
	ATOM 4949	CD1 LEUL 137	-4.769	53.275	76.806	1.00	6.19	C
	ATOM 4950	CD2 LEUL 137	-5.665	51.579	78.413	1.00	8.99	C
	ATOM 4951	N LEUL 138	-8.737	50.142	78.393	1.00	8.04	N
	ATOM 4952	CA LEUL 138	-9.232	50.068	79.754	1.00	7.27	C
	ATOM 4953	C LEUL 138	-7.971	50.062	80.604	1.00	8.18	C
	ATOM 4954	O LEUL 138	-7.334	49.024	80.787	1.00	9.08	O
	ATOM 4955	CB LEUL 138	-10.005	48.768	79.976	1.00	8.15	C
	ATOM 4956	CG LEUL 138	-11.401	48.604	79.373	1.00	6.72	C
	ATOM 4957	CD1 LEUL 138	-11.370	48.750	77.862	1.00	9.30	C
	ATOM 4958	CD2 LEUL 138	-11.918	47.243	79.753	1.00	7.37	C
	ATOM 4959	N ASN1 139	-7.588	51.225	81.107	1.00	10.27	N
	ATOM 4960	CA ASN1 139	-6.370	51.325	81.899	1.00	9.79	C
	ATOM 4961	C ASN1 139	-6.509	50.941	83.353	1.00	8.49	C
	ATOM 4962	O ASN1 139	-7.546	51.158	83.959	1.00	7.93	O
	ATOM 4963	CB ASN1 139	-5.770	52.725	81.795	1.00	11.38	C
	ATOM 4964	CG ASN1 139	-4.270	52.729	82.022	1.00	10.57	C
	ATOM 4965	OD1 ASN1 139	-3.524	52.111	81.271	1.00	10.47	O
	ATOM 4966	ND2 ASN1 139	-3.826	53.431	83.050	1.00	11.24	N
	ATOM 4967	N ASN1 140	-5.436	50.361	83.885	1.00	9.18	N
	ATOM 4968	CA ASN1 140	-5.316	49.910	85.278	1.00	8.78	C
	ATOM 4969	C ASN1 140	-6.577	49.542	86.049	1.00	8.46	C
	ATOM 4970	O ASN1 140	-7.055	50.321	86.885	1.00	7.23	O
	ATOM 4971	CB ASN1 140	-4.478	50.897	86.097	1.00	10.31	C
	ATOM 4972	CG ASN1 140	-3.059	51.042	85.564	1.00	13.49	C
	ATOM 4973	OD1 ASN1 140	-2.781	51.898	84.720	1.00	14.68	O
	ATOM 4974	ND2 ASN1 140	-2.155	50.207	86.055	1.00	16.04	N
	ATOM 4975	N PHEL 141	-7.103	48.354	85.760	1.00	8.17	N
	ATOM 4976	CA PHEL 141	-8.277	47.819	86.443	1.00	8.05	C
	ATOM 4977	C PHEL 141	-7.827	46.507	87.077	1.00	10.50	C
	ATOM 4978	O PHEL 141	-6.898	45.872	86.580	1.00	10.89	O
	ATOM 4979	CB PHEL 141	-9.446	47.599	85.476	1.00	7.55	C
	ATOM 4980	CG PHEL 141	-9.135	46.691	84.296	1.00	8.60	C
	ATOM 4981	CD1 PHEL 141	-8.330	47.126	83.254	1.00	9.02	C
	ATOM 4982	CD2 PHEL 141	-9.707	45.423	84.207	1.00	9.55	C
	ATOM 4983	CE1 PHEL 141	-8.092	46.313	82.138	1.00	11.26	C
	ATOM 4984	CE2 PHEL 141	-9.478	44.603	83.099	1.00	11.92	C
	ATOM 4985	CZ PHEL 141	-8.671	45.045	82.062	1.00	12.77	C
	ATOM 4986	N TYRL 142	-8.422	46.108	88.196	1.00	12.90	N
	ATOM 4987	CA TYRL 142	-7.972	44.863	88.810	1.00	13.83	C
	ATOM 4988	C TYRL 142	-8.500	43.532	88.249	1.00	16.80	C
	ATOM 4989	O TYRL 142	-7.765	42.848	87.529	1.00	19.27	O
	ATOM 4990	CB TYRL 142	-8.063	44.879	90.336	1.00	12.09	C
	ATOM 4991	CG TYRL 142	-7.711	43.522	90.898	1.00	9.68	C
	ATOM 4992	CD1 TYRL 142	-6.610	42.815	90.405	1.00	7.12	C
	ATOM 4993	CD2 TYRL 142	-8.546	42.886	91.806	1.00	9.85	C
	ATOM 4994	CE1 TYRL 142	-6.360	41.514	90.788	1.00	6.75	C
	ATOM 4995	CE2 TYRL 142	-8.298	41.578	92.201	1.00	11.16	C
	ATOM 4996	CZ TYRL 142	-7.207	40.896	91.682	1.00	7.17	C
	ATOM 4997	OH TYRL 142	-6.957	39.612	92.076	1.00	5.07	O
	ATOM 4998	N PRO1 143	-9.724	43.093	88.637	1.00	16.37	N
	ATOM 4999	CA PRO1 143	-10.134	41.815	88.050	1.00	15.10	C
	ATOM 5000	C PRO1 143	-9.923	41.889	86.557	1.00	15.25	C
	ATOM 5001	O PRO1 143	-10.364	42.850	85.914	1.00	13.71	O
	ATOM 5002	CB PRO1 143	-11.621	41.735	88.409	1.00	15.42	C
	ATOM 5003	CG PRO1 143	-11.692	42.422	89.725	1.00	15.74	C

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FIG. 53-79

ATOM 5005	N	ARGL 144	-9.111	40.959	86.056	1.00	17.00	N
ATOM 5006	CA	ARGL 144	-8.780	40.863	84.636	1.00	18.20	C
ATOM 5007	C	ARGL 144	-10.097	40.758	83.876	1.00	19.31	C
ATOM 5008	O	ARGL 144	-10.176	41.087	82.688	1.00	19.84	O
ATOM 5009	CB	ARGL 144	-7.909	39.624	84.393	1.00	19.37	C
ATOM 5010	CG	ARGL 144	-7.036	39.649	83.137	1.00	19.70	C
ATOM 5011	CD	ARGL 144	-6.209	38.359	83.032	1.00	18.40	C
ATOM 5012	NE	ARGL 144	-5.201	38.403	81.970	1.00	21.52	N
ATOM 5013	CZ	ARGL 144	-3.895	38.179	82.149	1.00	21.68	C
ATOM 5014	NH1	ARGL 144	-3.414	37.889	83.351	1.00	22.56	N
ATOM 5015	NH2	ARGL 144	-3.063	38.229	81.118	1.00	22.06	N
ATOM 5016	N	GLUL 145	-11.127	40.299	84.584	1.00	19.53	N
ATOM 5017	CA	GLUL 145	-12.464	40.159	84.030	1.00	20.80	C
ATOM 5018	C	GLUL 145	-13.128	41.510	83.690	1.00	21.40	C
ATOM 5019	O	GLUL 145	-13.634	42.235	84.566	1.00	20.44	O
ATOM 5020	CB	GLUL 145	-13.341	39.354	84.987	1.00	20.47	C
ATOM 5021	CG	GLUL 145	-12.988	37.874	85.071	1.00	21.37	C
ATOM 5022	CD	GLUL 145	-11.568	37.615	85.553	1.00	22.05	C
ATOM 5023	OE1	GLUL 145	-11.310	37.693	86.773	1.00	21.03	O
ATOM 5024	OE2	GLUL 145	-10.699	37.324	84.707	1.00	24.64	O
ATOM 5025	N	ALAL 146	-13.101	41.843	82.407	1.00	21.20	N
ATOM 5026	CA	ALAL 146	-13.701	43.066	81.913	1.00	21.63	C
ATOM 5027	C	ALAL 146	-14.450	42.732	80.621	1.00	23.24	C
ATOM 5028	O	ALAL 146	-14.173	41.717	79.974	1.00	23.86	O
ATOM 5029	CB	ALAL 146	-12.624	44.096	81.653	1.00	20.72	C
ATOM 5030	N	LYSL 147	-15.432	43.554	80.275	1.00	24.12	N
ATOM 5031	CA	LYSL 147	-16.201	43.348	79.057	1.00	24.43	C
ATOM 5032	C	LYSL 147	-15.997	44.575	78.183	1.00	25.90	C
ATOM 5033	O	LYSL 147	-15.704	45.671	78.680	1.00	26.11	O
ATOM 5034	CB	LYSL 147	-17.690	43.176	79.381	1.00	24.88	C
ATOM 5035	CG	LYSL 147	-18.431	42.127	78.535	1.00	23.00	C
ATOM 5036	CD	LYSL 147	-18.842	42.637	77.162	1.00	21.31	C
ATOM 5037	CE	LYSL 147	-19.490	41.519	76.353	1.00	21.90	C
ATOM 5038	NZ	LYSL 147	-19.871	41.911	74.964	1.00	19.83	N
ATOM 5039	N	VAL L 148	-16.111	44.370	76.875	1.00	26.98	N
ATOM 5040	CA	VAL L 148	-15.951	45.435	75.895	1.00	26.72	C
ATOM 5041	C	VAL L 148	-17.060	45.253	74.865	1.00	27.07	C
ATOM 5042	O	VAL L 148	-17.474	44.121	74.580	1.00	28.48	O
ATOM 5043	CB	VAL L 148	-14.581	45.337	75.170	1.00	25.94	C
ATOM 5044	CG1	VAL L 148	-14.311	46.595	74.394	1.00	24.38	C
ATOM 5045	CG2	VAL L 148	-13.454	45.064	76.161	1.00	24.31	C
ATOM 5046	N	GLNL 149	-17.588	46.360	74.361	1.00	26.55	N
ATOM 5047	CA	GLNL 149	-18.646	46.322	73.355	1.00	26.89	C
ATOM 5048	C	GLNL 149	-18.478	47.527	72.481	1.00	27.70	C
ATOM 5049	O	GLNL 149	-18.187	48.614	72.974	1.00	28.41	O
ATOM 5050	CB	GLNL 149	-20.025	46.377	73.996	1.00	26.69	C
ATOM 5051	CG	GLNL 149	-20.756	45.070	73.958	1.00	27.95	C
ATOM 5052	CD	GLNL 149	-21.890	45.024	74.947	1.00	30.34	C
ATOM 5053	OE1	GLNL 149	-21.723	44.573	76.086	1.00	30.41	O
ATOM 5054	NE2	GLNL 149	-23.056	45.471	74.520	1.00	31.39	N
ATOM 5055	N	TRPL 150	-18.611	47.331	71.179	1.00	27.58	N
ATOM 5056	CA	TRPL 150	-18.464	48.437	70.262	1.00	28.31	C
ATOM 5057	C	TRPL 150	-19.781	48.759	69.587	1.00	31.55	C
ATOM 5058	O	TRPL 150	-20.758	48.018	69.702	1.00	31.25	O
ATOM 5059	CB	TRPL 150	-17.403	48.130	69.209	1.00	23.64	C
ATOM 5060	CG	TRPL 150	-15.990	48.207	69.698	1.00	20.14	C
ATOM 5061	CD1	TRPL 150	-15.239	47.185	70.207	1.00	19.18	C
ATOM 5062	CD2	TRPL 150	-15.117	49.345	69.628	1.00	18.90	C
ATOM 5063	NE1	TRPL 150	-13.953	47.609	70.441	1.00	17.86	N
ATOM 5064	CE2	TRPL 150	-13.849	48.929	70.092	1.00	18.56	C
ATOM 5065	CE3	TRPL 150	-15.281	50.675	69.214	1.00	16.93	C
ATOM 5066	CZ2	TRPL 150	-12.753	49.798	70.154	1.00	17.58	C
ATOM 5067	CZ3	TRPL 150	-14.194	51.535	69.277	1.00	15.09	C
ATOM 5068	CH2	TRPL 150	-12.946	51.093	69.741	1.00	16.67	C
ATOM 5069	N	LYSL 151	-19.795	49.894	68.900	1.00	36.22	N
ATOM 5070	CA	LYSL 151	-20.952	50.362	68.159	1.00	39.51	C
ATOM 5071	C	LYSL 151	-20.340	50.949	66.888	1.00	41.77	C
ATOM 5072	O	LYSL 151	-19.170	51.349	66.876	1.00	42.22	O
ATOM 5073	CB	LYSL 151	-21.690	51.470	68.927	1.00	39.92	C
ATOM 5074	CG	LYSL 151	-21.854	51.720	70.476	1.00	43.00	C



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FIG. 53-80

ATOM 5076	CE LYS L 151	-24.384	51.432	70.668	1.00	47.81	C
ATOM 5077	NZ LYS L 151	-24.367	52.720	71.438	1.00	49.14	N
ATOM 5078	N VAL L 152	-21.106	50.920	65.805	1.00	43.46	N
ATOM 5079	CA VAL L 152	-20.665	51.476	64.531	1.00	43.64	C
ATOM 5080	C VAL L 152	-21.553	52.672	64.207	1.00	43.81	C
ATOM 5081	O VAL L 152	-21.213	53.495	63.354	1.00	43.94	O
ATOM 5082	CB VAL L 152	-20.795	50.445	63.390	1.00	44.47	C
ATOM 5083	CG1 VAL L 152	-22.265	50.156	63.094	1.00	44.41	C
ATOM 5084	CG2 VAL L 152	-20.068	50.941	62.145	1.00	45.11	C
ATOM 5085	N ASP L 153	-22.713	52.700	64.865	1.00	43.39	N
ATOM 5086	CA ASP L 153	-23.741	53.732	64.733	1.00	44.01	C
ATOM 5087	C ASP L 153	-24.910	53.233	65.574	1.00	44.62	C
ATOM 5088	O ASP L 153	-26.004	52.977	65.066	1.00	45.88	O
ATOM 5089	CB ASP L 153	-24.200	53.889	63.278	1.00	44.29	C
ATOM 5090	CG ASP L 153	-23.754	55.197	62.657	1.00	44.59	C
ATOM 5091	OD1 ASP L 153	-23.643	56.217	63.373	1.00	44.63	O
ATOM 5092	OD2 ASP L 153	-23.506	55.200	61.434	1.00	46.20	O
ATOM 5093	N ASN L 154	-24.635	53.004	66.853	1.00	43.73	N
ATOM 5094	CA ASN L 154	-25.623	52.504	67.808	1.00	42.71	C
ATOM 5095	C ASN L 154	-25.945	51.014	67.643	1.00	41.97	C
ATOM 5096	O ASN L 154	-26.535	50.405	68.534	1.00	41.18	O
ATOM 5097	CB ASN L 154	-26.909	53.342	67.784	1.00	43.27	C
ATOM 5098	CG ASN L 154	-27.507	53.523	69.171	1.00	43.36	C
ATOM 5099	OD1 ASN L 154	-26.791	53.492	70.182	1.00	44.42	O
ATOM 5100	ND2 ASN L 154	-28.816	53.735	69.227	1.00	41.84	N
ATOM 5101	N ALA L 155	-25.540	50.426	66.518	1.00	41.02	N
ATOM 5102	CA ALA L 155	-25.758	48.999	66.271	1.00	39.62	C
ATOM 5103	C ALA L 155	-24.522	48.263	66.787	1.00	38.90	C
ATOM 5104	O ALA L 155	-23.401	48.768	66.660	1.00	38.99	O
ATOM 5105	CB ALA L 155	-25.954	48.740	64.789	1.00	38.88	C
ATOM 5106	N LEU L 156	-24.719	47.073	67.347	1.00	38.28	N
ATOM 5107	CA LEU L 156	-23.619	46.294	67.916	1.00	37.65	C
ATOM 5108	C LEU L 156	-22.635	45.673	66.933	1.00	37.26	C
ATOM 5109	O LEU L 156	-23.020	45.233	65.848	1.00	37.41	O
ATOM 5110	CB LEU L 156	-24.163	45.216	68.859	1.00	36.83	C
ATOM 5111	CG LEU L 156	-23.847	45.405	70.346	1.00	34.02	C
ATOM 5112	CD1 LEU L 156	-22.342	45.392	70.532	1.00	33.39	C
ATOM 5113	CD2 LEU L 156	-24.442	46.710	70.867	1.00	32.28	C
ATOM 5114	N GLN L 157	-21.362	45.642	67.325	1.00	37.11	N
ATOM 5115	CA GLN L 157	-20.303	45.064	66.495	1.00	36.71	C
ATOM 5116	C GLN L 157	-19.739	43.792	67.115	1.00	36.12	C
ATOM 5117	O GLN L 157	-19.786	43.620	68.335	1.00	34.66	O
ATOM 5118	CB GLN L 157	-19.168	46.063	66.262	1.00	36.57	C
ATOM 5119	CG GLN L 157	-19.523	47.200	65.322	1.00	37.72	C
ATOM 5120	CD GLN L 157	-20.160	46.716	64.032	1.00	38.91	C
ATOM 5121	OE1 GLN L 157	-19.644	45.821	63.354	1.00	39.12	O
ATOM 5122	NE2 GLN L 157	-21.312	47.279	63.707	1.00	39.65	N
ATOM 5123	N SER L 158	-19.215	42.913	66.262	1.00	36.33	N
ATOM 5124	CA SER L 158	-18.639	41.639	66.680	1.00	35.62	C
ATOM 5125	C SER L 158	-17.820	41.000	65.558	1.00	35.19	C
ATOM 5126	O SER L 158	-18.158	41.122	64.382	1.00	35.02	O
ATOM 5127	CB SER L 158	-19.753	40.680	67.101	1.00	35.10	C
ATOM 5128	OG SER L 158	-20.726	40.548	66.077	1.00	32.12	O
ATOM 5129	N GLY L 159	-16.727	40.338	65.927	1.00	34.60	N
ATOM 5130	CA GLY L 159	-15.888	39.674	64.941	1.00	33.06	C
ATOM 5131	C GLY L 159	-14.677	40.454	64.472	1.00	32.15	C
ATOM 5132	O GLY L 159	-13.600	39.896	64.287	1.00	33.10	O
ATOM 5133	N ASN L 160	-14.843	41.757	64.307	1.00	31.89	N
ATOM 5134	CA ASN L 160	-13.754	42.612	63.836	1.00	30.85	C
ATOM 5135	C ASN L 160	-12.910	43.226	64.953	1.00	30.84	C
ATOM 5136	O ASN L 160	-11.991	44.010	64.684	1.00	30.24	O
ATOM 5137	CB ASN L 160	-14.314	43.709	62.931	1.00	30.08	C
ATOM 5138	CG ASN L 160	-15.620	44.263	63.440	1.00	29.11	C
ATOM 5139	OD1 ASN L 160	-15.864	44.285	64.648	1.00	28.52	O
ATOM 5140	ND2 ASN L 160	-16.486	44.673	62.528	1.00	29.91	N
ATOM 5141	N SER L 161	-13.208	42.861	66.198	1.00	30.23	N
ATOM 5142	CA SER L 161	-12.471	43.383	67.346	1.00	29.43	C
ATOM 5143	C SER L 161	-11.579	42.338	68.021	1.00	28.71	C
ATOM 5144	O SER L 161	-11.992	41.191	68.218	1.00	28.95	O
ATOM 5145	CB SER L 161	-12.440	42.004	68.352	1.00	29.60	C

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FIG. 53-81	ATOM 5147 N GLN L 162	-10.349	42.729	68.348	1.00	27.14	N
	ATOM 5148 CA GLN L 162	-9.402	41.829	69.010	1.00	26.44	C
	ATOM 5149 C GLN L 162	-8.672	42.481	70.187	1.00	26.49	C
	ATOM 5150 O GLN L 162	-7.754	43.297	70.002	1.00	26.77	O
	ATOM 5151 CB GLN L 162	-8.370	41.312	68.019	1.00	26.02	C
	ATOM 5152 CG GLN L 162	-8.906	40.359	66.992	1.00	24.83	C
	ATOM 5153 CD GLN L 162	-7.833	39.922	66.042	1.00	23.29	C
	ATOM 5154 OE1 GLN L 162	-7.586	40.574	65.031	1.00	24.66	O
	ATOM 5155 NE2 GLN L 162	-7.154	38.832	66.374	1.00	23.88	N
	ATOM 5156 N GLU L 163	-9.057	42.095	71.397	1.00	24.82	N
	ATOM 5157 CA GLU L 163	-8.436	42.650	72.583	1.00	23.67	C
	ATOM 5158 C GLU L 163	-7.177	41.949	73.039	1.00	21.69	C
	ATOM 5159 O GLU L 163	-6.864	40.835	72.615	1.00	21.45	O
	ATOM 5160 CB GLU L 163	-9.436	42.747	73.729	1.00	25.41	C
	ATOM 5161 CG GLU L 163	-10.291	41.535	73.934	1.00	29.25	C
	ATOM 5162 CD GLU L 163	-11.719	41.914	74.253	1.00	33.17	C
	ATOM 5163 OE1 GLU L 163	-12.315	42.680	73.456	1.00	34.01	O
	ATOM 5164 OE2 GLU L 163	-12.238	41.454	75.299	1.00	35.13	O
	ATOM 5165 N SER L 164	-6.444	42.636	73.900	1.00	19.82	N
	ATOM 5166 CA SER L 164	-5.206	42.129	74.453	1.00	17.86	C
	ATOM 5167 C SER L 164	-5.128	42.645	75.890	1.00	16.94	C
	ATOM 5168 O SER L 164	-5.679	43.706	76.203	1.00	19.26	O
	ATOM 5169 CB SER L 164	-4.033	42.647	73.619	1.00	16.64	C
	ATOM 5170 OG SER L 164	-2.828	42.015	73.990	1.00	19.50	O
	ATOM 5171 N VAL L 165	-4.505	41.875	76.772	1.00	14.24	N
	ATOM 5172 CA VAL L 165	-4.359	42.260	78.168	1.00	11.37	C
	ATOM 5173 C VAL L 165	-2.893	42.091	78.554	1.00	11.46	C
	ATOM 5174 O VAL L 165	-2.204	41.218	78.020	1.00	11.36	O
	ATOM 5175 CB VAL L 165	-5.243	41.383	79.078	1.00	9.55	C
	ATOM 5176 CG1 VAL L 165	-5.039	41.731	80.529	1.00	8.73	C
	ATOM 5177 CG2 VAL L 165	-6.693	41.574	78.723	1.00	11.84	C
	ATOM 5178 N THR L 166	-2.401	42.955	79.435	1.00	10.28	N
	ATOM 5179 CA THR L 166	-1.016	42.874	79.878	1.00	10.52	C
	ATOM 5180 C THR L 166	-0.858	41.859	81.020	1.00	12.19	C
	ATOM 5181 O THR L 166	-1.836	41.311	81.533	1.00	11.21	O
	ATOM 5182 CB THR L 166	-0.516	44.252	80.386	1.00	9.47	C
	ATOM 5183 OG1 THR L 166	-1.354	44.696	81.460	1.00	9.54	O
	ATOM 5184 CG2 THR L 166	-0.545	45.298	79.277	1.00	5.19	C
	ATOM 5185 N GLU L 167	0.383	41.534	81.351	1.00	14.91	N
	ATOM 5186 CA GLU L 167	0.645	40.645	82.473	1.00	17.53	C
	ATOM 5187 C GLU L 167	0.467	41.569	83.691	1.00	18.96	C
	ATOM 5188 O GLU L 167	0.747	42.766	83.603	1.00	20.99	O
	ATOM 5189 CB GLU L 167	2.079	40.104	82.413	1.00	19.23	C
	ATOM 5190 CG GLU L 167	2.337	39.039	81.343	1.00	22.37	C
	ATOM 5191 CD GLU L 167	1.759	37.676	81.701	1.00	25.92	C
	ATOM 5192 OE1 GLU L 167	1.837	37.279	82.888	1.00	27.11	O
	ATOM 5193 OE2 GLU L 167	1.223	37.000	80.792	1.00	26.04	O
	ATOM 5194 N GLN L 168	0.004	41.032	84.812	1.00	19.68	N
	ATOM 5195 CA GLN L 168	-0.225	41.832	86.016	1.00	20.51	C
	ATOM 5196 C GLN L 168	0.942	42.751	86.355	1.00	21.66	C
	ATOM 5197 O GLN L 168	2.096	42.322	86.312	1.00	21.63	O
	ATOM 5198 CB GLN L 168	-0.517	40.910	87.197	1.00	21.14	C
	ATOM 5199 CG GLN L 168	-0.921	41.622	88.455	1.00	19.06	C
	ATOM 5200 CD GLN L 168	-1.487	40.680	89.478	1.00	18.83	C
	ATOM 5201 OE1 GLN L 168	-0.861	39.681	89.841	1.00	17.90	O
	ATOM 5202 NE2 GLN L 168	-2.676	40.993	89.963	1.00	20.30	N
	ATOM 5203 N ASP L 169	0.635	44.003	86.709	1.00	22.03	N
	ATOM 5204 CA ASP L 169	1.682	44.972	87.033	1.00	22.10	C
	ATOM 5205 C ASP L 169	2.379	44.710	88.359	1.00	21.82	C
	ATOM 5206 O ASP L 169	1.735	44.432	89.378	1.00	21.33	O
	ATOM 5207 CB ASP L 169	1.171	46.413	86.978	1.00	23.06	C
	ATOM 5208 CG ASP L 169	2.313	47.422	86.896	1.00	24.41	C
	ATOM 5209 OD1 ASP L 169	2.862	47.788	87.953	1.00	27.41	O
	ATOM 5210 OD2 ASP L 169	2.716	47.804	85.776	1.00	22.98	O
	ATOM 5211 N SER L 170	3.703	44.840	88.329	1.00	22.45	N
	ATOM 5212 CA SER L 170	4.577	44.593	89.479	1.00	21.46	C
	ATOM 5213 C SER L 170	4.449	45.585	90.616	1.00	19.16	C
	ATOM 5214 O SER L 170	4.692	45.240	91.768	1.00	18.27	O
	ATOM 5215 CB SER L 170	6.037	44.511	89.022	1.00	22.76	C
	ATOM 5216 CG SER L 170	6.246	45.526	89.003	1.00	24.24	C

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FIG. 53-82	ATOM 5218	CA	LYSL 171	3.909	47.851	91.299	1.00	17.00	C
	ATOM 5219	C	LYSL 171	2.500	47.878	91.900	1.00	15.97	C
	ATOM 5220	O	LYSL 171	2.346	47.774	93.117	1.00	16.17	O
	ATOM 5221	CB	LYSL 171	4.248	49.231	90.722	1.00	17.18	C
	ATOM 5222	CG	LYSL 171	5.715	49.675	90.880	1.00	16.28	C
	ATOM 5223	CD	LYSL 171	6.701	48.884	90.022	1.00	16.75	C
	ATOM 5224	CE	LYSL 171	6.455	49.058	88.521	1.00	17.21	C
	ATOM 5225	NZ	LYSL 171	6.605	50.459	88.042	1.00	15.68	N
	ATOM 5226	N	ASPL 172	1.475	47.934	91.052	1.00	14.88	N
	ATOM 5227	CA	ASPL 172	0.101	48.028	91.542	1.00	15.20	C
	ATOM 5228	C	ASPL 172	-0.899	46.867	91.448	1.00	13.21	C
	ATOM 5229	O	ASPL 172	-2.074	47.033	91.801	1.00	11.47	O
	ATOM 5230	CB	ASPL 172	-0.544	49.330	91.032	1.00	20.61	C
	ATOM 5231	CG	ASPL 172	-0.329	49.581	89.533	1.00	24.63	C
	ATOM 5232	OD1	ASPL 172	0.829	49.697	89.086	1.00	26.58	O
	ATOM 5233	OD2	ASPL 172	-1.334	49.726	88.807	1.00	28.09	O
	ATOM 5234	N	SER L 173	-0.453	45.703	90.983	1.00	11.82	N
	ATOM 5235	CA	SER L 173	-1.313	44.520	90.875	1.00	9.20	C
	ATOM 5236	C	SER L 173	-2.608	44.676	90.071	1.00	9.25	C
	ATOM 5237	O	SER L 173	-3.592	43.976	90.323	1.00	11.51	O
	ATOM 5238	CB	SER L 173	-1.648	43.968	92.260	1.00	7.54	C
	ATOM 5239	OG	SER L 173	-0.472	43.679	92.991	1.00	4.68	O
	ATOM 5240	N	THRL 174	-2.600	45.570	89.093	1.00	7.82	N
	ATOM 5241	CA	THRL 174	-3.758	45.794	88.242	1.00	7.08	C
	ATOM 5242	C	THRL 174	-3.377	45.282	86.867	1.00	6.59	C
	ATOM 5243	O	THRL 174	-2.269	44.775	86.696	1.00	7.57	O
	ATOM 5244	CB	THRL 174	-4.112	47.289	88.155	1.00	8.05	C
	ATOM 5245	OG1	THRL 174	-2.999	48.019	87.622	1.00	6.17	O
	ATOM 5246	CG2	THRL 174	-4.459	47.833	89.533	1.00	7.23	C
	ATOM 5247	N	TYRL 175	-4.294	45.385	85.909	1.00	6.94	N
	ATOM 5248	CA	TYRL 175	-4.075	44.947	84.522	1.00	9.29	C
	ATOM 5249	C	TYRL 175	-4.596	46.049	83.608	1.00	9.75	C
	ATOM 5250	O	TYRL 175	-5.155	47.039	84.071	1.00	9.70	O
	ATOM 5251	CB	TYRL 175	-4.906	43.694	84.199	1.00	10.57	C
	ATOM 5252	CG	TYRL 175	-4.476	42.417	84.857	1.00	11.63	C
	ATOM 5253	CD1	TYRL 175	-3.547	41.589	84.249	1.00	12.07	C
	ATOM 5254	CD2	TYRL 175	-5.007	42.025	86.087	1.00	15.20	C
	ATOM 5255	CE1	TYRL 175	-3.152	40.404	84.841	1.00	13.77	C
	ATOM 5256	CE2	TYRL 175	-4.614	40.831	86.693	1.00	14.73	C
	ATOM 5257	CZ	TYRL 175	-3.688	40.030	86.057	1.00	14.27	C
	ATOM 5258	OH	TYRL 175	-3.301	38.844	86.619	1.00	18.68	O
	ATOM 5259	N	SER L 176	-4.462	45.852	82.306	1.00	11.16	N
	ATOM 5260	CA	SER L 176	-4.985	46.803	81.337	1.00	11.52	C
	ATOM 5261	C	SER L 176	-5.392	46.037	80.090	1.00	12.38	C
	ATOM 5262	O	SER L 176	-4.954	44.910	79.886	1.00	11.64	O
	ATOM 5263	CB	SER L 176	-3.969	47.890	81.036	1.00	11.51	C
	ATOM 5264	OG	SER L 176	-3.744	48.662	82.210	1.00	14.01	O
	ATOM 5265	N	LEUL 177	-6.274	46.611	79.284	1.00	16.50	N
	ATOM 5266	CA	LEUL 177	-6.749	45.928	78.075	1.00	18.46	C
	ATOM 5267	C	LEUL 177	-6.842	46.873	76.893	1.00	18.55	C
	ATOM 5268	O	LEUL 177	-7.090	48.069	77.063	1.00	19.01	O
	ATOM 5269	CB	LEUL 177	-8.126	45.291	78.342	1.00	19.24	C
	ATOM 5270	CG	LEUL 177	-8.809	44.351	77.334	1.00	19.52	C
	ATOM 5271	CD1	LEUL 177	-9.779	43.441	78.058	1.00	16.66	C
	ATOM 5272	CD2	LEUL 177	-9.528	45.125	76.248	1.00	19.49	C
	ATOM 5273	N	SER L 178	-6.616	46.348	75.699	1.00	18.94	N
	ATOM 5274	CA	SER L 178	-6.713	47.173	74.508	1.00	20.49	C
	ATOM 5275	C	SER L 178	-7.591	46.468	73.495	1.00	20.65	C
	ATOM 5276	O	SER L 178	-7.305	45.332	73.099	1.00	19.96	O
	ATOM 5277	CB	SER L 178	-5.337	47.463	73.906	1.00	21.19	C
	ATOM 5278	OG	SER L 178	-4.732	46.293	73.384	1.00	23.79	O
	ATOM 5279	N	SER L 179	-8.708	47.101	73.150	1.00	20.87	N
	ATOM 5280	CA	SER L 179	-9.613	46.528	72.179	1.00	20.29	C
	ATOM 5281	C	SER L 179	-9.659	47.394	70.938	1.00	19.00	C
	ATOM 5282	O	SER L 179	-10.183	48.502	70.965	1.00	20.70	O
	ATOM 5283	CB	SER L 179	-11.011	46.344	72.757	1.00	20.27	C
	ATOM 5284	OG	SER L 179	-11.775	45.498	71.908	1.00	23.08	O
	ATOM 5285	N	THRL 180	-9.062	46.883	69.869	1.00	16.84	N
	ATOM 5286	CA	THRL 180	-9.000	47.541	68.570	1.00	14.41	C
	ATOM 5287	C	THRL 180	-10.151	47.047	67.604	1.00	15.07	C

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FIG. 53-83	ATOM 5289	CB THRL 180	-7.708	47.142	67.872	1.00	10.71	C
	ATOM 5290	OG1 THRL 180	-6.640	47.187	68.822	1.00	6.75	O
	ATOM 5291	CG2 THRL 180	-7.404	48.071	66.701	1.00	9.72	C
	ATOM 5292	N LEUL 181	-10.787	47.966	66.956	1.00	13.84	N
	ATOM 5293	CA LEUL 181	-11.886	47.610	66.051	1.00	12.92	C
	ATOM 5294	C LEUL 181	-11.428	47.989	64.666	1.00	12.23	C
	ATOM 5295	O LEUL 181	-11.007	49.109	64.460	1.00	13.31	O
	ATOM 5296	CB LEUL 181	-13.173	48.369	66.377	1.00	12.17	C
	ATOM 5297	CG LEUL 181	-14.419	47.790	65.692	1.00	13.24	C
	ATOM 5298	CD1 LEUL 181	-14.774	46.483	66.366	1.00	14.73	C
	ATOM 5299	CD2 LEUL 181	-15.603	48.732	65.753	1.00	10.88	C
	ATOM 5300	N THRL 182	-11.523	47.074	63.710	1.00	14.78	N
	ATOM 5301	CA THRL 182	-11.065	47.377	62.362	1.00	17.68	C
	ATOM 5302	C THRL 182	-12.143	47.375	61.277	1.00	20.12	C
	ATOM 5303	O THRL 182	-13.009	46.486	61.221	1.00	20.43	O
	ATOM 5304	CB THRL 182	-9.922	46.434	61.929	1.00	17.07	C
	ATOM 5305	OG1 THRL 182	-9.398	45.753	63.078	1.00	19.00	O
	ATOM 5306	CG2 THRL 182	-8.799	47.237	61.279	1.00	15.70	C
	ATOM 5307	N LEUL 183	-12.082	48.401	60.433	1.00	19.48	N
	ATOM 5308	CA LEUL 183	-12.994	48.570	59.315	1.00	20.51	C
	ATOM 5309	C LEUL 183	-12.102	49.119	58.208	1.00	21.81	C
	ATOM 5310	O LEUL 183	-11.075	49.747	58.489	1.00	22.53	O
	ATOM 5311	CB LEUL 183	-14.074	49.617	59.626	1.00	21.14	C
	ATOM 5312	CG LEUL 183	-14.678	49.864	61.016	1.00	22.09	C
	ATOM 5313	CD1 LEUL 183	-13.813	50.846	61.819	1.00	21.67	C
	ATOM 5314	CD2 LEUL 183	-16.069	50.460	60.835	1.00	22.48	C
	ATOM 5315	N SERL 184	-12.450	48.865	56.952	1.00	23.13	N
	ATOM 5316	CA SERL 184	-11.647	49.403	55.859	1.00	24.35	C
	ATOM 5317	C SERL 184	-11.875	50.911	55.867	1.00	25.23	C
	ATOM 5318	O SERL 184	-12.862	51.383	56.441	1.00	23.92	O
	ATOM 5319	CB SERL 184	-12.076	48.811	54.507	1.00	23.84	C
	ATOM 5320	OG SERL 184	-13.421	49.132	54.177	1.00	22.29	O
	ATOM 5321	N LYSL 185	-10.960	51.664	55.262	1.00	27.81	N
	ATOM 5322	CA LYSL 185	-11.097	53.121	55.176	1.00	29.86	C
	ATOM 5323	C LYSL 185	-12.488	53.424	54.636	1.00	30.28	C
	ATOM 5324	O LYSL 185	-13.128	54.395	55.034	1.00	29.66	O
	ATOM 5325	CB LYSL 185	-10.063	53.688	54.201	1.00	31.37	C
	ATOM 5326	CG LYSL 185	-10.308	55.121	53.777	1.00	32.79	C
	ATOM 5327	CD LYSL 185	-9.946	56.088	54.873	1.00	34.93	C
	ATOM 5328	CE LYSL 185	-10.021	57.528	54.374	1.00	37.29	C
	ATOM 5329	NZ LYSL 185	-9.371	57.706	53.053	1.00	38.05	N
	ATOM 5330	N ALAL 186	-12.941	52.562	53.730	1.00	30.68	N
	ATOM 5331	CA ALAL 186	-14.247	52.697	53.123	1.00	30.54	C
	ATOM 5332	C ALAL 186	-15.360	52.612	54.175	1.00	30.37	C
	ATOM 5333	O ALAL 186	-15.930	53.637	54.540	1.00	29.84	O
	ATOM 5334	CB ALAL 186	-14.425	51.644	52.045	1.00	31.15	C
	ATOM 5335	N ASPL 187	-15.604	51.425	54.730	1.00	30.03	N
	ATOM 5336	CA ASPL 187	-16.672	51.269	55.722	1.00	30.35	C
	ATOM 5337	C ASPL 187	-16.644	52.238	56.895	1.00	29.09	C
	ATOM 5338	O ASPL 187	-17.659	52.427	57.563	1.00	28.33	O
	ATOM 5339	CB ASPL 187	-16.791	49.834	56.245	1.00	32.83	C
	ATOM 5340	CG ASPL 187	-18.020	49.646	57.136	1.00	35.98	C
	ATOM 5341	OD1 ASPL 187	-19.134	50.044	56.714	1.00	37.38	O
	ATOM 5342	OD2 ASPL 187	-17.872	49.139	58.273	1.00	37.57	O
	ATOM 5343	N TYRL 188	-15.487	52.832	57.172	1.00	28.85	N
	ATOM 5344	CA TYRL 188	-15.403	53.804	58.257	1.00	28.55	C
	ATOM 5345	C TYRL 188	-16.148	55.027	57.750	1.00	29.22	C
	ATOM 5346	O TYRL 188	-17.145	55.456	58.338	1.00	28.87	O
	ATOM 5347	CB TYRL 188	-13.952	54.171	58.562	1.00	26.77	C
	ATOM 5348	CG TYRL 188	-13.789	54.987	59.819	1.00	23.61	C
	ATOM 5349	CD1 TYRL 188	-13.874	54.388	61.074	1.00	23.89	C
	ATOM 5350	CD2 TYRL 188	-13.541	56.351	59.760	1.00	24.55	C
	ATOM 5351	CE1 TYRL 188	-13.718	55.131	62.242	1.00	22.87	C
	ATOM 5352	CE2 TYRL 188	-13.379	57.109	60.925	1.00	23.85	C
	ATOM 5353	CZ TYRL 188	-13.469	56.492	62.161	1.00	24.60	C
	ATOM 5354	OH TYRL 188	-13.294	57.221	63.314	1.00	25.17	O
	ATOM 5355	N GLUL 189	-15.679	55.551	56.621	1.00	30.25	N
	ATOM 5356	CA GLUL 189	-16.294	56.709	55.989	1.00	31.78	C
	ATOM 5357	C GLUL 189	-17.635	56.234	55.427	1.00	32.83	C
	ATOM 5358	O GLUL 189	-17.751	55.861	54.953	1.00	33.41	O

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FIG. 53-84	ATOM 5360 CG GLUL 189	-14.039	57.792	55.365	1.00	35.25	C
	ATOM 5361 CD GLUL 189	-13.155	58.303	54.227	1.00	38.13	C
	ATOM 5362 OE1 GLUL 189	-12.850	57.522	53.286	1.00	38.01	O
	ATOM 5363 OE2 GLUL 189	-12.735	59.482	54.280	1.00	37.07	O
	ATOM 5364 N LYS L 190	-18.629	56.202	56.308	1.00	33.88	N
	ATOM 5365 CA LYS L 190	-19.982	55.765	55.984	1.00	35.62	C
	ATOM 5366 C LYS L 190	-20.819	55.887	57.240	1.00	36.04	C
	ATOM 5367 O LYS L 190	-22.023	56.113	57.180	1.00	35.82	O
	ATOM 5368 CB LYS L 190	-19.988	54.298	55.552	1.00	37.09	C
	ATOM 5369 CG LYS L 190	-21.375	53.697	55.331	1.00	39.08	C
	ATOM 5370 CD LYS L 190	-21.263	52.280	54.793	1.00	39.92	C
	ATOM 5371 CE LYS L 190	-22.619	51.693	54.452	1.00	40.51	C
	ATOM 5372 NZ LYS L 190	-23.432	51.415	55.662	1.00	41.41	N
	ATOM 5373 N HIS L 191	-20.175	55.696	58.382	1.00	36.86	N
	ATOM 5374 CA HIS L 191	-20.867	55.765	59.651	1.00	38.35	C
	ATOM 5375 C HIS L 191	-20.559	57.060	60.375	1.00	38.02	C
	ATOM 5376 O HIS L 191	-19.904	57.946	59.811	1.00	38.09	O
	ATOM 5377 CB HIS L 191	-20.515	54.547	60.496	1.00	41.04	C
	ATOM 5378 CG HIS L 191	-20.845	53.250	59.827	1.00	43.74	C
	ATOM 5379 ND1 HIS L 191	-21.990	52.534	60.109	1.00	45.64	N
	ATOM 5380 CD2 HIS L 191	-20.188	52.546	58.876	1.00	44.80	C
	ATOM 5381 CE1 HIS L 191	-22.019	51.443	59.364	1.00	46.20	C
	ATOM 5382 NE2 HIS L 191	-20.936	51.428	58.605	1.00	46.13	N
	ATOM 5383 N LYS L 192	-21.049	57.180	61.606	1.00	37.21	N
	ATOM 5384 CA LYS L 192	-20.834	58.391	62.379	1.00	35.55	C
	ATOM 5385 C LYS L 192	-20.311	58.150	63.784	1.00	34.21	C
	ATOM 5386 O LYS L 192	-19.176	58.517	64.080	1.00	33.55	O
	ATOM 5387 CB LYS L 192	-22.129	59.206	62.453	1.00	36.25	C
	ATOM 5388 CG LYS L 192	-21.924	60.697	62.642	1.00	36.77	C
	ATOM 5389 CD LYS L 192	-21.449	61.346	61.354	1.00	38.24	C
	ATOM 5390 CE LYS L 192	-21.185	62.828	61.534	1.00	38.31	C
	ATOM 5391 NZ LYS L 192	-20.072	63.050	62.495	1.00	39.59	N
	ATOM 5392 N VAL L 193	-21.130	57.540	64.643	1.00	33.66	N
	ATOM 5393 CA VAL L 193	-20.753	57.306	66.042	1.00	33.51	C
	ATOM 5394 C VAL L 193	-20.094	55.977	66.405	1.00	32.45	C
	ATOM 5395 O VAL L 193	-20.729	54.917	66.369	1.00	33.05	O
	ATOM 5396 CB VAL L 193	-21.947	57.577	67.014	1.00	34.88	C
	ATOM 5397 CG1 VAL L 193	-23.222	56.937	66.500	1.00	36.25	C
	ATOM 5398 CG2 VAL L 193	-21.632	57.050	68.406	1.00	34.56	C
	ATOM 5399 N TYR L 194	-18.837	56.066	66.837	1.00	30.50	N
	ATOM 5400 CA TYR L 194	-18.056	54.906	67.239	1.00	29.68	C
	ATOM 5401 C TYR L 194	-17.936	54.879	68.756	1.00	28.79	C
	ATOM 5402 O TYR L 194	-17.132	55.612	69.340	1.00	28.23	O
	ATOM 5403 CB TYR L 194	-16.677	54.952	66.585	1.00	30.77	C
	ATOM 5404 CG TYR L 194	-16.752	54.849	65.082	1.00	31.80	C
	ATOM 5405 CD1 TYR L 194	-16.927	53.614	64.460	1.00	33.05	C
	ATOM 5406 CD2 TYR L 194	-16.710	55.990	64.283	1.00	32.55	C
	ATOM 5407 CE1 TYR L 194	-17.066	53.517	63.076	1.00	34.52	C
	ATOM 5408 CE2 TYR L 194	-16.847	55.906	62.901	1.00	33.29	C
	ATOM 5409 CZ TYR L 194	-17.026	54.667	62.303	1.00	34.31	C
	ATOM 5410 OH TYR L 194	-17.166	54.567	60.939	1.00	35.51	O
	ATOM 5411 N ALA L 195	-18.738	54.024	69.387	1.00	28.06	N
	ATOM 5412 CA ALA L 195	-18.762	53.909	70.844	1.00	26.33	C
	ATOM 5413 C ALA L 195	-18.081	52.676	71.419	1.00	24.97	C
	ATOM 5414 O ALA L 195	-18.228	51.566	70.916	1.00	23.70	O
	ATOM 5415 CB ALA L 195	-20.195	53.984	71.349	1.00	26.18	C
	ATOM 5416 N CYS L 196	-17.356	52.900	72.507	1.00	24.91	N
	ATOM 5417 CA CYS L 196	-16.644	51.857	73.230	1.00	23.12	C
	ATOM 5418 C CYS L 196	-17.325	51.725	74.582	1.00	22.46	C
	ATOM 5419 O CYS L 196	-17.170	52.594	75.432	1.00	21.59	O
	ATOM 5420 CB CYS L 196	-15.177	52.259	73.437	1.00	21.41	C
	ATOM 5421 SG CYS L 196	-14.373	51.154	74.618	1.00	22.26	S
	ATOM 5422 N GLUL 197	-18.143	50.692	74.743	1.00	24.50	N
	ATOM 5423 CA GLUL 197	-18.865	50.443	75.993	1.00	26.84	C
	ATOM 5424 C GLUL 197	-18.065	49.467	76.837	1.00	26.75	C
	ATOM 5425 O GLUL 197	-17.591	48.453	76.325	1.00	26.00	O
	ATOM 5426 CB GLUL 197	-20.259	49.861	75.707	1.00	29.41	C
	ATOM 5427 CG GLUL 197	-21.032	49.408	76.951	1.00	32.09	C
	ATOM 5428 CD GLUL 197	-22.365	48.731	76.627	1.00	35.08	C
	ATOM 5429 OE1 GLUL 189	-22.626	48.226	75.402	1.00	33.57	O

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FIG. 53-85	ATOM 5431 N VALL 198	-17.925	49.775	78.125	1.00	27.83	N
	ATOM 5432 CA VALL 198	-17.165	48.936	79.048	1.00	28.59	C
	ATOM 5433 C VALL 198	-17.918	48.592	80.336	1.00	28.86	C
	ATOM 5434 O VALL 198	-18.672	49.413	80.864	1.00	28.87	O
	ATOM 5435 CB VALL 198	-15.834	49.610	79.441	1.00	29.04	C
	ATOM 5436 CG1 VALL 198	-15.016	48.672	80.323	1.00	30.38	C
	ATOM 5437 CG2 VALL 198	-15.046	50.012	78.192	1.00	27.67	C
	ATOM 5438 N THRL 199	-17.681	47.386	80.850	1.00	29.52	N
	ATOM 5439 CA THRL 199	-18.316	46.906	82.080	1.00	29.04	C
	ATOM 5440 C THRL 199	-17.256	46.289	83.013	1.00	29.21	C
	ATOM 5441 O THRL 199	-16.282	45.691	82.547	1.00	29.24	O
	ATOM 5442 CB THRL 199	-19.381	45.852	81.759	1.00	28.14	C
	ATOM 5443 OG1 THRL 199	-20.075	46.226	80.562	1.00	25.12	O
	ATOM 5444 CG2 THRL 199	-20.374	45.750	82.894	1.00	27.36	C
	ATOM 5445 N HISL 200	-17.459	46.400	84.323	1.00	28.56	N
	ATOM 5446 CA HISL 200	-16.486	45.884	85.291	1.00	28.22	C
	ATOM 5447 C HISL 200	-17.031	46.131	86.697	1.00	29.26	C
	ATOM 5448 O HISL 200	-18.082	46.755	86.845	1.00	30.25	O
	ATOM 5449 CB HISL 200	-15.165	46.659	85.114	1.00	26.36	C
	ATOM 5450 CG HISL 200	-14.007	46.097	85.878	1.00	24.47	C
	ATOM 5451 ND1 HISL 200	-13.423	46.756	86.936	1.00	25.60	N
	ATOM 5452 CD2 HISL 200	-13.296	44.958	85.711	1.00	24.69	C
	ATOM 5453 CE1 HISL 200	-12.404	46.052	87.386	1.00	24.64	C
	ATOM 5454 NE2 HISL 200	-12.304	44.955	86.659	1.00	24.23	N
	ATOM 5455 N GLNL 201	-16.382	45.568	87.718	1.00	30.03	N
	ATOM 5456 CA GLNL 201	-16.793	45.834	89.102	1.00	31.30	C
	ATOM 5457 C GLNL 201	-16.113	47.175	89.326	1.00	30.74	C
	ATOM 5458 O GLNL 201	-15.063	47.435	88.734	1.00	31.30	O
	ATOM 5459 CB GLNL 201	-16.189	44.837	90.098	1.00	32.87	C
	ATOM 5460 CG GLNL 201	-16.631	43.395	89.984	1.00	36.94	C
	ATOM 5461 CD GLNL 201	-16.046	42.536	91.100	1.00	39.17	C
	ATOM 5462 OE1 GLNL 201	-15.413	41.511	90.850	1.00	42.29	O
	ATOM 5463 NE2 GLNL 201	-16.245	42.964	92.336	1.00	38.36	N
	ATOM 5464 N GLYL 202	-16.673	48.027	90.168	1.00	30.22	N
	ATOM 5465 CA GLYL 202	-16.042	49.318	90.386	1.00	28.92	C
	ATOM 5466 C GLYL 202	-16.707	50.315	89.463	1.00	27.74	C
	ATOM 5467 O GLYL 202	-17.014	51.434	89.877	1.00	27.84	O
	ATOM 5468 N LEUL 203	-16.879	49.928	88.200	1.00	26.12	N
	ATOM 5469 CA LEUL 203	-17.573	50.770	87.239	1.00	25.22	C
	ATOM 5470 C LEUL 203	-19.024	50.467	87.547	1.00	26.14	C
	ATOM 5471 O LEUL 203	-19.561	49.448	87.111	1.00	27.79	O
	ATOM 5472 CB LEUL 203	-17.263	50.379	85.789	1.00	22.88	C
	ATOM 5473 CG LEUL 203	-15.948	50.884	85.186	1.00	22.14	C
	ATOM 5474 CD1 LEUL 203	-15.916	50.610	83.697	1.00	20.58	C
	ATOM 5475 CD2 LEUL 203	-15.794	52.371	85.446	1.00	22.72	C
	ATOM 5476 N SERL 204	-19.600	51.299	88.404	1.00	26.56	N
	ATOM 5477 CA SERL 204	-20.985	51.187	88.853	1.00	26.25	C
	ATOM 5478 C SERL 204	-21.965	50.924	87.700	1.00	27.59	C
	ATOM 5479 O SERL 204	-22.775	49.987	87.750	1.00	28.27	O
	ATOM 5480 CB SERL 204	-21.355	52.472	89.599	1.00	25.01	C
	ATOM 5481 OG SERL 204	-20.257	53.382	89.615	1.00	18.30	O
	ATOM 5482 N SERL 205	-21.880	51.759	86.668	1.00	27.10	N
	ATOM 5483 CA SERL 205	-22.721	51.638	85.486	1.00	26.02	C
	ATOM 5484 C SERL 205	-21.739	51.597	84.310	1.00	26.45	C
	ATOM 5485 O SERL 205	-20.614	52.096	84.418	1.00	27.30	O
	ATOM 5486 CB SERL 205	-23.647	52.858	85.362	1.00	25.69	C
	ATOM 5487 OG SERL 205	-24.017	53.391	86.631	1.00	24.11	O
	ATOM 5488 N PROL 206	-22.132	50.972	83.189	1.00	25.99	N
	ATOM 5489 CA PROL 206	-21.263	50.877	82.011	1.00	25.85	C
	ATOM 5490 C PROL 206	-20.719	52.224	81.541	1.00	25.60	C
	ATOM 5491 O PROL 206	-21.465	53.202	81.430	1.00	25.34	O
	ATOM 5492 CB PROL 206	-22.183	50.243	80.969	1.00	25.19	C
	ATOM 5493 CG PROL 206	-23.020	49.324	81.803	1.00	25.62	C
	ATOM 5494 CD PROL 206	-23.375	50.208	82.981	1.00	26.67	C
	ATOM 5495 N VALL 207	-19.413	52.267	81.286	1.00	25.53	N
	ATOM 5496 CA VALL 207	-18.744	53.479	80.821	1.00	25.91	C
	ATOM 5497 C VALL 207	-18.592	53.451	79.304	1.00	25.77	C
	ATOM 5498 O VALL 207	-18.041	52.509	78.724	1.00	23.99	O
	ATOM 5499 CB VALL 207	-17.353	53.664	81.482	1.00	26.93	C
	ATOM 5500 CG1 VALL 207	-16.640	54.867	80.000	1.00	28.46	C

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FIG. 53-86

ATOM 5502	N	THR L 208	-19.104	54.488	78.663	1.00	26.57	N
ATOM 5503	CA	THR L 208	-19.037	54.580	77.223	1.00	26.91	C
ATOM 5504	C	THR L 208	-18.158	55.756	76.827	1.00	26.87	C
ATOM 5505	O	THR L 208	-18.326	56.876	77.318	1.00	26.95	O
ATOM 5506	CB	THR L 208	-20.457	54.749	76.599	1.00	27.63	C
ATOM 5507	OG1	THR L 208	-21.355	53.779	77.163	1.00	27.17	O
ATOM 5508	CG2	THR L 208	-20.399	54.543	75.089	1.00	25.39	C
ATOM 5509	N	LYS L 209	-17.176	55.473	75.985	1.00	26.18	N
ATOM 5510	CA	LYS L 209	-16.266	56.484	75.481	1.00	24.86	C
ATOM 5511	C	LYS L 209	-16.485	56.409	73.989	1.00	25.02	C
ATOM 5512	O	LYS L 209	-16.110	55.428	73.356	1.00	24.92	O
ATOM 5513	CB	LYS L 209	-14.825	56.134	75.847	1.00	23.11	C
ATOM 5514	CG	LYS L 209	-14.557	56.159	77.349	1.00	20.42	C
ATOM 5515	CD	LYS L 209	-14.713	57.547	77.918	1.00	16.39	C
ATOM 5516	CE	LYS L 209	-14.289	57.597	79.379	1.00	15.96	C
ATOM 5517	NZ	LYS L 209	-14.204	58.997	79.884	1.00	13.55	N
ATOM 5518	N	SER L 210	-17.164	57.417	73.451	1.00	26.26	N
ATOM 5519	CA	SER L 210	-17.495	57.454	72.035	1.00	25.99	C
ATOM 5520	C	SER L 210	-17.085	58.749	71.346	1.00	25.10	C
ATOM 5521	O	SER L 210	-16.750	59.737	71.998	1.00	24.15	O
ATOM 5522	CB	SER L 210	-19.006	57.245	71.885	1.00	26.74	C
ATOM 5523	OG	SER L 210	-19.410	57.220	70.532	1.00	29.39	O
ATOM 5524	N	PHE L 211	-17.118	58.723	70.018	1.00	25.06	N
ATOM 5525	CA	PHE L 211	-16.792	59.884	69.202	1.00	24.49	C
ATOM 5526	C	PHE L 211	-17.575	59.847	67.887	1.00	25.43	C
ATOM 5527	O	PHE L 211	-18.606	59.171	67.794	1.00	24.52	O
ATOM 5528	CB	PHE L 211	-15.281	60.005	68.967	1.00	22.18	C
ATOM 5529	CG	PHE L 211	-14.722	58.992	68.019	1.00	19.69	C
ATOM 5530	CD1	PHE L 211	-14.587	57.666	68.399	1.00	22.38	C
ATOM 5531	CD2	PHE L 211	-14.299	59.375	66.754	1.00	19.66	C
ATOM 5532	CE1	PHE L 211	-14.035	56.730	67.532	1.00	23.82	C
ATOM 5533	CE2	PHE L 211	-13.748	58.458	65.880	1.00	21.68	C
ATOM 5534	CZ	PHE L 211	-13.613	57.128	66.265	1.00	23.57	C
ATOM 5535	N	ASN L 212	-17.088	60.543	66.864	1.00	27.12	N
ATOM 5536	CA	ASN L 212	-17.804	60.589	65.599	1.00	29.02	C
ATOM 5537	C	ASN L 212	-16.968	61.048	64.412	1.00	29.36	C
ATOM 5538	O	ASN L 212	-15.887	61.620	64.577	1.00	30.52	O
ATOM 5539	CB	ASN L 212	-19.020	61.506	65.739	1.00	30.60	C
ATOM 5540	CG	ASN L 212	-18.664	62.839	66.362	1.00	33.09	C
ATOM 5541	OD1	ASN L 212	-17.724	63.509	65.931	1.00	34.33	O
ATOM 5542	ND2	ASN L 212	-19.391	63.218	67.398	1.00	34.80	N
ATOM 5543	N	ARG L 213	-17.523	60.819	63.221	1.00	28.51	N
ATOM 5544	CA	ARG L 213	-16.925	61.172	61.937	1.00	27.37	C
ATOM 5545	C	ARG L 213	-15.935	60.112	61.479	1.00	27.24	C
ATOM 5546	O	ARG L 213	-16.182	59.572	60.379	1.00	26.68	O
ATOM 5547	CB	ARG L 213	-16.256	62.552	61.974	1.00	27.60	C
ATOM 5548	CG	ARG L 213	-17.211	63.732	62.152	1.00	27.69	C
ATOM 5549	CD	ARG L 213	-16.461	65.073	62.178	1.00	28.10	C
ATOM 5550	NE	ARG L 213	-15.404	65.092	63.188	1.00	27.20	N
ATOM 5551	CZ	ARG L 213	-14.103	65.179	62.917	1.00	26.87	C
ATOM 5552	NH1	ARG L 213	-13.687	65.262	61.659	1.00	24.89	N
ATOM 5553	NH2	ARG L 213	-13.217	65.159	63.906	1.00	27.14	N
TER 5554		ARG L 213						
ATOM 5555	N	GLN H 1	26.213	20.467	86.642	1.00	30.62	N
ATOM 5556	CA	GLN H 1	25.208	21.506	86.279	1.00	30.11	C
ATOM 5557	C	GLN H 1	25.492	21.995	84.875	1.00	28.53	C
ATOM 5558	O	GLN H 1	26.450	22.733	84.656	1.00	28.92	O
ATOM 5559	CB	GLN H 1	25.284	22.688	87.245	1.00	31.70	C
ATOM 5560	CG	GLN H 1	24.677	22.432	88.599	1.00	34.69	C
ATOM 5561	CD	GLN H 1	23.178	22.640	88.612	1.00	37.49	C
ATOM 5562	OE1	GLN H 1	22.661	23.538	87.960	1.00	39.94	O
ATOM 5563	NE2	GLN H 1	22.474	21.822	89.375	1.00	39.50	N
ATOM 5564	N	VAL H 2	24.684	21.565	83.915	1.00	27.15	N
ATOM 5565	CA	VAL H 2	24.884	21.992	82.538	1.00	25.30	C
ATOM 5566	C	VAL H 2	24.331	23.394	82.259	1.00	24.46	C
ATOM 5567	O	VAL H 2	23.586	23.958	83.071	1.00	24.66	O
ATOM 5568	CB	VAL H 2	24.296	20.980	81.522	1.00	25.51	C
ATOM 5569	CG1	VAL H 2	25.240	19.807	81.343	1.00	26.22	C
ATOM 5570	CG2	VAL H 2	22.941	20.493	81.976	1.00	26.52	C
ATOM 5571	N	GLN H 2	24.718	22.053	81.115	1.00	22.32	N

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FIG. 53-87

ATOM 5573	C	GLNH	3	23.779	25.101	79.264	1.00	17.85	C
ATOM 5574	O	GLNH	3	24.567	24.928	78.334	1.00	18.21	O
ATOM 5575	CB	GLNH	3	25.440	26.249	80.707	1.00	24.73	C
ATOM 5576	CG	GLNH	3	25.999	26.486	82.097	1.00	31.68	C
ATOM 5577	CD	GLNH	3	24.952	27.019	83.053	1.00	35.61	C
ATOM 5578	OE1	GLNH	3	23.968	27.638	82.635	1.00	37.48	O
ATOM 5579	NE2	GLNH	3	25.150	26.777	84.346	1.00	37.34	N
ATOM 5580	N	LEUH	4	22.463	25.105	79.110	1.00	15.92	N
ATOM 5581	CA	LEUH	4	21.837	24.915	77.806	1.00	13.88	C
ATOM 5582	C	LEUH	4	21.557	26.214	77.063	1.00	12.34	C
ATOM 5583	O	LEUH	4	20.797	27.057	77.543	1.00	12.85	O
ATOM 5584	CB	LEUH	4	20.527	24.134	77.966	1.00	12.78	C
ATOM 5585	CG	LEUH	4	20.551	22.875	78.841	1.00	10.51	C
ATOM 5586	CD1	LEUH	4	19.148	22.302	78.905	1.00	8.09	C
ATOM 5587	CD2	LEUH	4	21.549	21.852	78.295	1.00	10.28	C
ATOM 5588	N	LEUH	5	22.163	26.354	75.887	1.00	10.72	N
ATOM 5589	CA	LEUH	5	21.986	27.528	75.036	1.00	8.44	C
ATOM 5590	C	LEUH	5	21.508	27.034	73.676	1.00	7.46	C
ATOM 5591	O	LEUH	5	22.153	26.180	73.057	1.00	8.22	O
ATOM 5592	CB	LEUH	5	23.298	28.324	74.910	1.00	8.68	C
ATOM 5593	CG	LEUH	5	24.595	27.587	74.551	1.00	7.55	C
ATOM 5594	CD1	LEUH	5	25.538	28.507	73.816	1.00	8.28	C
ATOM 5595	CD2	LEUH	5	25.265	27.009	75.796	1.00	10.07	C
ATOM 5596	N	GLUH	6	20.398	27.597	73.204	1.00	7.38	N
ATOM 5597	CA	GLUH	6	19.775	27.192	71.938	1.00	6.70	C
ATOM 5598	C	GLUH	6	19.929	28.157	70.771	1.00	7.54	C
ATOM 5599	O	GLUH	6	20.386	29.287	70.941	1.00	8.78	O
ATOM 5600	CB	GLUH	6	18.294	26.930	72.181	1.00	3.52	C
ATOM 5601	CG	GLUH	6	18.038	26.284	73.528	1.00	3.07	C
ATOM 5602	CD	GLUH	6	16.636	25.803	73.690	1.00	2.00	C
ATOM 5603	OE1	GLUH	6	16.043	25.332	72.704	1.00	2.00	O
ATOM 5604	OE2	GLUH	6	16.127	25.889	74.819	1.00	2.00	O
ATOM 5605	N	SERH	7	19.510	27.706	69.592	1.00	7.96	N
ATOM 5606	CA	SERH	7	19.582	28.492	68.364	1.00	8.44	C
ATOM 5607	C	SERH	7	18.514	29.581	68.321	1.00	8.77	C
ATOM 5608	O	SERH	7	17.502	29.486	69.008	1.00	9.13	O
ATOM 5609	CB	SERH	7	19.467	27.569	67.143	1.00	11.38	C
ATOM 5610	OG	SERH	7	18.512	26.535	67.352	1.00	15.43	O
ATOM 5611	N	GLYH	8	18.739	30.601	67.495	1.00	7.57	N
ATOM 5612	CA	GLYH	8	17.814	31.717	67.394	1.00	6.97	C
ATOM 5613	C	GLYH	8	16.500	31.345	66.762	1.00	5.80	C
ATOM 5614	O	GLYH	8	16.328	30.200	66.365	1.00	6.19	O
ATOM 5615	N	ALAH	9	15.607	32.321	66.613	1.00	4.10	N
ATOM 5616	CA	ALAH	9	14.288	32.082	66.037	1.00	5.03	C
ATOM 5617	C	ALAH	9	14.295	31.591	64.581	1.00	5.79	C
ATOM 5618	O	ALAH	9	15.226	31.874	63.821	1.00	7.48	O
ATOM 5619	CB	ALAH	9	13.452	33.315	66.165	1.00	4.80	C
ATOM 5620	N	GLUH	10	13.237	30.883	64.198	1.00	3.83	N
ATOM 5621	CA	GLUH	10	13.104	30.333	62.851	1.00	3.26	C
ATOM 5622	C	GLUH	10	11.787	30.743	62.232	1.00	3.25	C
ATOM 5623	O	GLUH	10	10.751	30.728	62.887	1.00	5.55	O
ATOM 5624	CB	GLUH	10	13.109	28.795	62.885	1.00	3.97	C
ATOM 5625	CG	GLUH	10	14.443	28.128	63.180	1.00	2.24	C
ATOM 5626	CD	GLUH	10	15.375	28.103	61.997	1.00	2.00	C
ATOM 5627	OE1	GLUH	10	14.933	28.232	60.830	1.00	3.34	O
ATOM 5628	OE2	GLUH	10	16.575	27.925	62.232	1.00	3.37	O
ATOM 5629	N	VALH	11	11.809	31.072	60.953	1.00	3.17	N
ATOM 5630	CA	VALH	11	10.591	31.433	60.252	1.00	5.01	C
ATOM 5631	C	VALH	11	10.587	30.415	59.122	1.00	4.61	C
ATOM 5632	O	VALH	11	11.561	30.328	58.373	1.00	3.89	O
ATOM 5633	CB	VALH	11	10.642	32.875	59.699	1.00	8.53	C
ATOM 5634	CG1	VALH	11	9.238	33.342	59.344	1.00	7.21	C
ATOM 5635	CG2	VALH	11	11.277	33.814	60.724	1.00	9.48	C
ATOM 5636	N	LYSH	12	9.545	29.587	59.072	1.00	4.07	N
ATOM 5637	CA	LYSH	12	9.420	28.538	58.072	1.00	5.19	C
ATOM 5638	C	LYSH	12	8.045	28.563	57.420	1.00	5.91	C
ATOM 5639	O	LYSH	12	7.065	28.902	58.077	1.00	8.34	O
ATOM 5640	CB	LYSH	12	9.576	27.166	58.752	1.00	5.83	C
ATOM 5641	CG	LYSH	12	10.920	26.885	59.393	1.00	2.00	C
ATOM 5642	CD	LYSH	12	12.010	26.774	58.773	1.00	2.00	C



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FIG. 53-88	ATOM 5644	NZ LYSH 12	14.489	26.810	58.321	1.00	6.51	N
	ATOM 5645	N LYSH 13	7.956	28.202	56.142	1.00	5.24	N
	ATOM 5646	CA LYSH 13	6.646	28.152	55.486	1.00	6.75	C
	ATOM 5647	C LYSH 13	6.097	26.765	55.855	1.00	6.71	C
	ATOM 5648	O LYSH 13	6.868	25.824	56.060	1.00	6.69	O
	ATOM 5649	CB LYSH 13	6.762	28.264	53.955	1.00	7.21	C
	ATOM 5650	CG LYSH 13	7.358	29.558	53.391	1.00	5.94	C
	ATOM 5651	CD LYSH 13	6.434	30.739	53.593	1.00	9.27	C
	ATOM 5652	CE LYSH 13	6.696	31.844	52.586	1.00	8.08	C
	ATOM 5653	NZ LYSH 13	6.285	31.389	51.234	1.00	14.24	N
	ATOM 5654	N PROH 14	4.768	26.613	55.945	1.00	6.24	N
	ATOM 5655	CA PROH 14	4.247	25.288	56.301	1.00	5.61	C
	ATOM 5656	C PROH 14	4.558	24.213	55.263	1.00	5.99	C
	ATOM 5657	O PROH 14	4.224	24.341	54.089	1.00	6.85	O
	ATOM 5658	CB PROH 14	2.746	25.537	56.486	1.00	7.13	C
	ATOM 5659	CG PROH 14	2.475	26.763	55.637	1.00	7.66	C
	ATOM 5660	CD PROH 14	3.690	27.613	55.843	1.00	5.62	C
	ATOM 5661	N GLYH 15	5.231	23.160	55.712	1.00	6.24	N
	ATOM 5662	CA GLYH 15	5.608	22.066	54.836	1.00	3.56	C
	ATOM 5663	C GLYH 15	7.106	21.841	54.889	1.00	3.60	C
	ATOM 5664	O GLYH 15	7.603	20.830	54.392	1.00	4.72	O
	ATOM 5665	N SERH 16	7.811	22.756	55.548	1.00	3.55	N
	ATOM 5666	CA SERH 16	9.268	22.716	55.670	1.00	4.48	C
	ATOM 5667	C SERH 16	9.789	21.893	56.857	1.00	6.62	C
	ATOM 5668	O SERH 16	9.007	21.347	57.645	1.00	7.95	O
	ATOM 5669	CB SERH 16	9.798	24.155	55.759	1.00	4.84	C
	ATOM 5670	OG SERH 16	9.098	25.014	54.867	1.00	2.00	O
	ATOM 5671	N SERH 17	11.112	21.778	56.952	1.00	8.11	N
	ATOM 5672	CA SERH 17	11.766	21.033	58.026	1.00	9.36	C
	ATOM 5673	C SERH 17	12.585	22.002	58.861	1.00	10.49	C
	ATOM 5674	O SERH 17	13.310	22.845	58.324	1.00	13.72	O
	ATOM 5675	CB SERH 17	12.731	19.984	57.463	1.00	8.58	C
	ATOM 5676	OG SERH 17	12.092	19.077	56.583	1.00	11.68	O
	ATOM 5677	N VALH 18	12.514	21.853	60.173	1.00	9.20	N
	ATOM 5678	CA VALH 18	13.254	22.722	61.063	1.00	8.05	C
	ATOM 5679	C VALH 18	14.114	21.868	61.970	1.00	10.27	C
	ATOM 5680	O VALH 18	13.706	20.780	62.387	1.00	9.51	O
	ATOM 5681	CB VALH 18	12.311	23.587	61.923	1.00	7.91	C
	ATOM 5682	CG1 VALH 18	11.629	22.743	63.029	1.00	3.28	C
	ATOM 5683	CG2 VALH 18	13.076	24.759	62.496	1.00	8.24	C
	ATOM 5684	N LYSH 19	15.323	22.346	62.235	1.00	12.29	N
	ATOM 5685	CA LYSH 19	16.249	21.645	63.101	1.00	13.79	C
	ATOM 5686	C LYSH 19	16.826	22.678	64.039	1.00	14.54	C
	ATOM 5687	O LYSH 19	17.589	23.554	63.612	1.00	15.89	O
	ATOM 5688	CB LYSH 19	17.373	20.970	62.299	1.00	14.50	C
	ATOM 5689	CG LYSH 19	18.479	20.367	63.172	1.00	15.10	C
	ATOM 5690	CD LYSH 19	19.433	19.495	62.392	1.00	13.35	C
	ATOM 5691	CE LYSH 19	19.050	18.028	62.523	1.00	18.64	C
	ATOM 5692	NZ LYSH 19	17.755	17.668	61.866	1.00	23.12	N
	ATOM 5693	N VALH 20	16.423	22.594	65.304	1.00	13.54	N
	ATOM 5694	CA VALH 20	16.892	23.518	66.334	1.00	11.88	C
	ATOM 5695	C VALH 20	17.949	22.804	67.177	1.00	9.59	C
	ATOM 5696	O VALH 20	17.826	21.609	67.399	1.00	10.23	O
	ATOM 5697	CB VALH 20	15.703	23.993	67.191	1.00	12.27	C
	ATOM 5698	CG1 VALH 20	14.670	24.674	66.298	1.00	9.57	C
	ATOM 5699	CG2 VALH 20	15.054	22.818	67.887	1.00	13.94	C
	ATOM 5700	N SERH 21	19.004	23.510	67.581	1.00	7.81	N
	ATOM 5701	CA SERH 21	20.091	22.917	68.370	1.00	6.84	C
	ATOM 5702	C SERH 21	20.080	23.367	69.816	1.00	6.68	C
	ATOM 5703	O SERH 21	19.492	24.392	70.147	1.00	8.90	O
	ATOM 5704	CB SERH 21	21.465	23.253	67.765	1.00	7.77	C
	ATOM 5705	OG SERH 21	21.991	24.507	68.211	1.00	6.16	O
	ATOM 5706	N CYSH 22	20.836	22.670	70.653	1.00	6.28	N
	ATOM 5707	CA CYSH 22	20.903	22.996	72.069	1.00	7.75	C
	ATOM 5708	C CYSH 22	22.274	22.607	72.618	1.00	7.86	C
	ATOM 5709	O CYSH 22	22.495	21.456	73.001	1.00	8.34	O
	ATOM 5710	CB CYSH 22	19.800	22.244	72.803	1.00	10.65	C
	ATOM 5711	SG CYSH 22	19.857	22.267	74.625	1.00	16.65	S
	ATOM 5712	N LYSH 23	23.193	23.571	72.627	1.00	8.06	N
	ATOM 5713	CA LYSH 23	24.550	23.250	73.101	1.00	8.11	C

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FIG. 53-89	ATOM 5715 O LYSH 23	24.416	24.136	75.376	1.00	10.29	O
	ATOM 5716 CB LYSH 23	25.436	24.538	72.675	1.00	6.14	C
	ATOM 5717 CG LYSH 23	26.885	24.185	72.370	1.00	6.72	C
	ATOM 5718 CD LYSH 23	26.982	23.294	71.141	1.00	9.64	C
	ATOM 5719 CE LYSH 23	26.287	23.912	69.927	1.00	11.78	C
	ATOM 5720 NZ LYSH 23	26.297	23.010	68.743	1.00	10.31	N
	ATOM 5721 N ALAH 24	24.925	21.955	75.054	1.00	8.98	N
	ATOM 5722 CA ALAH 24	25.049	21.619	76.476	1.00	9.53	C
	ATOM 5723 C ALAH 24	26.497	21.789	76.937	1.00	10.70	C
	ATOM 5724 O ALAH 24	27.420	21.260	76.330	1.00	11.55	O
	ATOM 5725 CB ALAH 24	24.595	20.195	76.720	1.00	7.15	C
	ATOM 5726 N SERH 25	26.698	22.515	78.023	1.00	12.78	N
	ATOM 5727 CA SERH 25	28.044	22.742	78.518	1.00	14.78	C
	ATOM 5728 C SERH 25	28.071	22.741	80.033	1.00	14.58	C
	ATOM 5729 O SERH 25	27.024	22.852	80.662	1.00	13.09	O
	ATOM 5730 CB SERH 25	28.574	24.069	77.972	1.00	17.62	C
	ATOM 5731 OG SERH 25	27.614	25.105	78.103	1.00	22.32	O
	ATOM 5732 N GLYH 26	29.255	22.541	80.608	1.00	15.92	N
	ATOM 5733 CA GLYH 26	29.396	22.548	82.056	1.00	17.21	C
	ATOM 5734 C GLYH 26	29.420	21.220	82.795	1.00	18.55	C
	ATOM 5735 O GLYH 26	29.938	21.141	83.910	1.00	19.33	O
	ATOM 5736 N ASPH 27	28.901	20.164	82.182	1.00	19.59	N
	ATOM 5737 CA ASPH 27	28.867	18.862	82.841	1.00	20.42	C
	ATOM 5738 C ASPH 27	28.865	17.725	81.824	1.00	19.89	C
	ATOM 5739 O ASPH 27	28.167	17.816	80.806	1.00	20.24	O
	ATOM 5740 CB ASPH 27	27.592	18.764	83.690	1.00	21.74	C
	ATOM 5741 CG ASPH 27	27.873	18.502	85.152	1.00	22.03	C
	ATOM 5742 OD1 ASPH 27	28.419	19.391	85.833	1.00	25.42	O
	ATOM 5743 OD2 ASPH 27	27.509	17.421	85.648	1.00	24.27	O
	ATOM 5744 N THR H 28	29.630	16.665	82.109	1.00	18.47	N
	ATOM 5745 CA THR H 28	29.729	15.460	81.265	1.00	15.68	C
	ATOM 5746 C THR H 28	28.413	15.173	80.540	1.00	15.10	C
	ATOM 5747 O THR H 28	27.528	14.503	81.074	1.00	16.73	O
	ATOM 5748 CB THR H 28	30.057	14.197	82.110	1.00	14.61	C
	ATOM 5749 OG1 THR H 28	31.190	14.438	82.948	1.00	16.36	O
	ATOM 5750 CG2 THR H 28	30.371	13.026	81.212	1.00	13.15	C
	ATOM 5751 N PHEH 29	28.332	15.643	79.303	1.00	13.46	N
	ATOM 5752 CA PHEH 29	27.159	15.511	78.437	1.00	13.09	C
	ATOM 5753 C PHEH 29	26.405	14.179	78.469	1.00	13.89	C
	ATOM 5754 O PHEH 29	25.177	14.171	78.561	1.00	13.56	O
	ATOM 5755 CB PHEH 29	27.585	15.838	76.998	1.00	13.57	C
	ATOM 5756 CG PHEH 29	26.467	15.823	75.991	1.00	10.76	C
	ATOM 5757 CD1 PHEH 29	25.376	16.670	76.125	1.00	12.04	C
	ATOM 5758 CD2 PHEH 29	26.555	15.028	74.858	1.00	11.09	C
	ATOM 5759 CE1 PHEH 29	24.396	16.734	75.140	1.00	10.05	C
	ATOM 5760 CE2 PHEH 29	25.579	15.083	73.867	1.00	10.65	C
	ATOM 5761 CZ PHEH 29	24.498	15.943	74.010	1.00	11.71	C
	ATOM 5762 N ILEH 30	27.143	13.070	78.394	1.00	14.74	N
	ATOM 5763 CA ILEH 30	26.554	11.724	78.367	1.00	14.10	C
	ATOM 5764 C ILEH 30	25.740	11.336	79.583	1.00	13.21	C
	ATOM 5765 O ILEH 30	24.757	10.593	79.460	1.00	12.68	O
	ATOM 5766 CB ILEH 30	27.614	10.606	78.183	1.00	15.32	C
	ATOM 5767 CG1 ILEH 30	29.008	11.088	78.599	1.00	17.77	C
	ATOM 5768 CG2 ILEH 30	27.552	10.049	76.781	1.00	15.71	C
	ATOM 5769 CD1 ILEH 30	30.129	10.067	78.345	1.00	19.27	C
	ATOM 5770 N ARGH 31	26.148	11.847	80.746	1.00	10.64	N
	ATOM 5771 CA ARGH 31	25.494	11.545	82.022	1.00	6.72	C
	ATOM 5772 C ARGH 31	24.125	12.200	82.201	1.00	4.71	C
	ATOM 5773 O ARGH 31	23.568	12.151	83.288	1.00	4.96	O
	ATOM 5774 CB ARGH 31	26.398	11.978	83.181	1.00	6.64	C
	ATOM 5775 CG ARGH 31	27.847	11.483	83.120	1.00	7.34	C
	ATOM 5776 CD ARGH 31	28.625	11.984	84.345	1.00	11.53	C
	ATOM 5777 NE ARGH 31	30.059	11.651	84.342	1.00	12.07	N
	ATOM 5778 CZ ARGH 31	30.604	10.661	85.054	1.00	12.53	C
	ATOM 5779 NH1 ARGH 31	29.837	9.899	85.819	1.00	10.53	N
	ATOM 5780 NH2 ARGH 31	31.919	10.447	85.028	1.00	11.18	N
	ATOM 5781 N TYRH 32	23.589	12.794	81.138	1.00	3.90	N
	ATOM 5782 CA TYRH 32	22.309	13.493	81.157	1.00	2.81	C
	ATOM 5783 C TYRH 32	21.437	12.987	80.023	1.00	3.71	C
	ATOM 5784 O TYRH 32	21.061	12.487	79.017	1.00	3.40	O

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FIG. 53-90	ATOM 5786	CG TYR H 32	23.120	15.821	82.001	1.00	7.39	C
	ATOM 5787	CD1 TYR H 32	24.490	15.803	82.281	1.00	6.34	C
	ATOM 5788	CD2 TYR H 32	22.299	16.630	82.781	1.00	6.97	C
	ATOM 5789	CE1 TYR H 32	25.017	16.571	83.318	1.00	10.53	C
	ATOM 5790	CE2 TYR H 32	22.802	17.395	83.806	1.00	10.74	C
	ATOM 5791	CZ TYR H 32	24.158	17.373	84.086	1.00	13.42	C
	ATOM 5792	OH TYR H 32	24.619	18.143	85.144	1.00	15.09	O
	ATOM 5793	N SER H 33	20.117	13.129	80.173	1.00	3.85	N
	ATOM 5794	CA SER H 33	19.182	12.755	79.113	1.00	5.31	C
	ATOM 5795	C SER H 33	18.376	14.012	78.804	1.00	6.65	C
	ATOM 5796	O SER H 33	17.848	14.648	79.718	1.00	6.29	O
	ATOM 5797	CB SER H 33	18.280	11.591	79.521	1.00	5.99	C
	ATOM 5798	OG SER H 33	17.341	11.937	80.508	1.00	3.85	O
	ATOM 5799	N PHE H 34	18.315	14.391	77.530	1.00	7.73	N
	ATOM 5800	CA PHE H 34	17.611	15.610	77.126	1.00	7.57	C
	ATOM 5801	C PHE H 34	16.258	15.426	76.464	1.00	7.43	C
	ATOM 5802	O PHE H 34	16.065	14.551	75.626	1.00	8.72	O
	ATOM 5803	CB PHE H 34	18.518	16.478	76.268	1.00	7.39	C
	ATOM 5804	CG PHE H 34	19.806	16.826	76.941	1.00	7.62	C
	ATOM 5805	CD1 PHE H 34	19.878	17.891	77.820	1.00	8.01	C
	ATOM 5806	CD2 PHE H 34	20.939	16.053	76.730	1.00	8.52	C
	ATOM 5807	CE1 PHE H 34	21.057	18.194	78.477	1.00	8.53	C
	ATOM 5808	CE2 PHE H 34	22.122	16.345	77.382	1.00	8.34	C
	ATOM 5809	CZ PHE H 34	22.179	17.413	78.259	1.00	9.73	C
	ATOM 5810	N THR H 35	15.345	16.316	76.827	1.00	8.01	N
	ATOM 5811	CA THR H 35	13.976	16.310	76.361	1.00	8.74	C
	ATOM 5812	C THR H 35	13.682	17.643	75.691	1.00	10.09	C
	ATOM 5813	O THR H 35	14.391	18.635	75.906	1.00	11.27	O
	ATOM 5814	CB THR H 35	13.018	16.195	77.571	1.00	9.79	C
	ATOM 5815	OG1 THR H 35	13.450	15.141	78.441	1.00	9.92	O
	ATOM 5816	CG2 THR H 35	11.596	15.916	77.116	1.00	9.69	C
	ATOM 5817	N TRP H 36	12.627	17.664	74.885	1.00	9.20	N
	ATOM 5818	CA TRP H 36	12.198	18.874	74.210	1.00	7.34	C
	ATOM 5819	C TRP H 36	10.757	19.148	74.605	1.00	7.87	C
	ATOM 5820	O TRP H 36	9.906	18.247	74.563	1.00	8.30	O
	ATOM 5821	CB TRP H 36	12.318	18.732	72.700	1.00	4.76	C
	ATOM 5822	CG TRP H 36	13.720	18.892	72.206	1.00	3.17	C
	ATOM 5823	CD1 TRP H 36	14.635	17.904	71.996	1.00	2.08	C
	ATOM 5824	CD2 TRP H 36	14.366	20.119	71.848	1.00	3.73	C
	ATOM 5825	NE1 TRP H 36	15.808	18.433	71.525	1.00	2.00	N
	ATOM 5826	CE2 TRP H 36	15.674	19.793	71.422	1.00	4.34	C
	ATOM 5827	CE3 TRP H 36	13.965	21.464	71.836	1.00	2.18	C
	ATOM 5828	CZ2 TRP H 36	16.595	20.769	70.994	1.00	3.76	C
	ATOM 5829	CZ3 TRP H 36	14.881	22.436	71.409	1.00	3.07	C
	ATOM 5830	CH2 TRP H 36	16.178	22.079	70.990	1.00	2.86	C
	ATOM 5831	N VAL H 37	10.513	20.376	75.059	1.00	7.63	N
	ATOM 5832	CA VAL H 37	9.193	20.824	75.474	1.00	6.92	C
	ATOM 5833	C VAL H 37	8.840	22.050	74.630	1.00	7.51	C
	ATOM 5834	O VAL H 37	9.632	22.988	74.522	1.00	6.76	O
	ATOM 5835	CB VAL H 37	9.174	21.206	76.978	1.00	6.04	C
	ATOM 5836	CG1 VAL H 37	7.813	21.754	77.371	1.00	5.15	C
	ATOM 5837	CG2 VAL H 37	9.507	19.999	77.834	1.00	5.87	C
	ATOM 5838	N ARG H 38	7.677	22.010	73.989	1.00	8.71	N
	ATOM 5839	CA ARG H 38	7.211	23.119	73.148	1.00	7.89	C
	ATOM 5840	C ARG H 38	6.103	23.862	73.865	1.00	8.66	C
	ATOM 5841	O ARG H 38	5.390	23.288	74.703	1.00	8.92	O
	ATOM 5842	CB ARG H 38	6.678	22.613	71.795	1.00	5.20	C
	ATOM 5843	CG ARG H 38	5.619	21.528	71.910	1.00	4.10	C
	ATOM 5844	CD ARG H 38	4.557	21.585	70.810	1.00	2.00	C
	ATOM 5845	NE ARG H 38	5.067	21.324	69.467	1.00	5.03	N
	ATOM 5846	CZ ARG H 38	4.311	20.873	68.466	1.00	5.96	C
	ATOM 5847	NH1 ARG H 38	3.020	20.616	68.660	1.00	5.70	N
	ATOM 5848	NH2 ARG H 38	4.823	20.763	67.250	1.00	2.54	N
	ATOM 5849	N GLN H 39	5.947	25.136	73.531	1.00	9.12	N
	ATOM 5850	CA GLN H 39	4.904	25.946	74.149	1.00	9.49	C
	ATOM 5851	C GLN H 39	4.377	26.934	73.125	1.00	10.88	C
	ATOM 5852	O GLN H 39	5.129	27.747	72.588	1.00	11.68	O
	ATOM 5853	CB GLN H 39	5.451	26.680	75.365	1.00	7.51	C
	ATOM 5854	CG GLN H 39	4.394	27.331	76.241	1.00	6.05	C
	ATOM 5855	CD GLN H 39	5.015	28.003	77.282	1.00	2.75	C

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FIG. 53-91	ATOM 5857 NE2 GLNH 39	4.335	28.135	78.517	1.00	4.69	N
	ATOM 5858 N ALAH 40	3.102	26.783	72.789	1.00	11.12	N
	ATOM 5859 CA ALAH 40	2.451	27.648	71.832	1.00	11.60	C
	ATOM 5860 C ALAH 40	2.036	28.922	72.551	1.00	12.54	C
	ATOM 5861 O ALAH 40	1.617	28.878	73.711	1.00	11.95	O
	ATOM 5862 CB ALAH 40	1.227	26.946	71.257	1.00	12.94	C
	ATOM 5863 N PROH 41	2.122	30.073	71.863	1.00	13.85	N
	ATOM 5864 CA PROH 41	1.776	31.406	72.355	1.00	14.71	C
	ATOM 5865 C PROH 41	0.992	31.547	73.659	1.00	16.10	C
	ATOM 5866 O PROH 41	1.566	31.942	74.684	1.00	16.71	O
	ATOM 5867 CB PROH 41	1.047	31.993	71.165	1.00	14.20	C
	ATOM 5868 CG PROH 41	1.977	31.579	70.052	1.00	15.51	C
	ATOM 5869 CD PROH 41	2.453	30.154	70.429	1.00	13.73	C
	ATOM 5870 N GLYH 42	-0.303	31.241	73.634	1.00	16.21	N
	ATOM 5871 CA GLYH 42	-1.095	31.387	74.845	1.00	17.00	C
	ATOM 5872 C GLYH 42	-1.464	30.098	75.545	1.00	16.65	C
	ATOM 5873 O GLYH 42	-2.388	30.074	76.376	1.00	15.76	O
	ATOM 5874 N GLNH 43	-0.738	29.031	75.223	1.00	15.80	N
	ATOM 5875 CA GLNH 43	-1.003	27.719	75.811	1.00	15.55	C
	ATOM 5876 C GLNH 43	0.085	27.280	76.791	1.00	13.04	C
	ATOM 5877 O GLNH 43	0.962	28.067	77.167	1.00	13.60	O
	ATOM 5878 CB GLNH 43	-1.159	26.669	74.708	1.00	17.67	C
	ATOM 5879 CG GLNH 43	-2.090	27.079	73.597	1.00	23.37	C
	ATOM 5880 CD GLNH 43	-3.421	27.567	74.120	1.00	29.07	C
	ATOM 5881 OE1 GLNH 43	-3.669	28.773	74.190	1.00	32.20	O
	ATOM 5882 NE2 GLNH 43	-4.291	26.634	74.490	1.00	32.38	N
	ATOM 5883 N GLYH 44	0.013	26.020	77.204	1.00	9.85	N
	ATOM 5884 CA GLYH 44	0.979	25.486	78.136	1.00	7.51	C
	ATOM 5885 C GLYH 44	2.035	24.598	77.514	1.00	6.25	C
	ATOM 5886 O GLYH 44	2.139	24.495	76.284	1.00	4.79	O
	ATOM 5887 N LEUH 45	2.809	23.952	78.387	1.00	5.54	N
	ATOM 5888 CA LEUH 45	3.897	23.050	78.011	1.00	4.49	C
	ATOM 5889 C LEUH 45	3.410	21.717	77.419	1.00	4.02	C
	ATOM 5890 O LEUH 45	2.361	21.209	77.813	1.00	3.67	O
	ATOM 5891 CB LEUH 45	4.752	22.761	79.243	1.00	4.27	C
	ATOM 5892 CG LEUH 45	5.391	23.917	80.015	1.00	2.21	C
	ATOM 5893 CD1 LEUH 45	5.956	23.392	81.334	1.00	2.00	C
	ATOM 5894 CD2 LEUH 45	6.477	24.576	79.193	1.00	2.87	C
	ATOM 5895 N GLUH 46	4.177	21.175	76.476	1.00	3.36	N
	ATOM 5896 CA GLUH 46	3.873	19.902	75.813	1.00	4.62	C
	ATOM 5897 C GLUH 46	5.141	19.074	75.579	1.00	4.79	C
	ATOM 5898 O GLUH 46	6.088	19.519	74.917	1.00	5.47	O
	ATOM 5899 CB GLUH 46	3.179	20.128	74.461	1.00	5.98	C
	ATOM 5900 CG GLUH 46	3.287	18.939	73.500	1.00	2.77	C
	ATOM 5901 CD GLUH 46	2.415	19.066	72.264	1.00	2.40	C
	ATOM 5902 OE1 GLUH 46	1.191	19.249	72.407	1.00	2.00	O
	ATOM 5903 OE2 GLUH 46	2.945	18.947	71.139	1.00	3.18	O
	ATOM 5904 N TRPH 47	5.140	17.860	76.110	1.00	4.47	N
	ATOM 5905 CA TRPH 47	6.264	16.947	75.972	1.00	4.38	C
	ATOM 5906 C TRPH 47	6.284	16.461	74.521	1.00	4.97	C
	ATOM 5907 O TRPH 47	5.256	16.006	74.005	1.00	5.28	O
	ATOM 5908 CB TRPH 47	6.054	15.767	76.933	1.00	6.19	C
	ATOM 5909 CG TRPH 47	7.283	14.946	77.262	1.00	7.45	C
	ATOM 5910 CD1 TRPH 47	8.253	15.249	78.182	1.00	6.44	C
	ATOM 5911 CD2 TRPH 47	7.672	13.694	76.664	1.00	4.88	C
	ATOM 5912 NE1 TRPH 47	9.220	14.263	78.186	1.00	6.10	N
	ATOM 5913 CE2 TRPH 47	8.890	13.302	77.266	1.00	2.74	C
	ATOM 5914 CE3 TRPH 47	7.117	12.871	75.677	1.00	5.15	C
	ATOM 5915 CZ2 TRPH 47	9.559	12.131	76.907	1.00	2.54	C
	ATOM 5916 CZ3 TRPH 47	7.787	11.700	75.320	1.00	3.52	C
	ATOM 5917 CH2 TRPH 47	8.994	11.345	75.934	1.00	3.72	C
	ATOM 5918 N METH 48	7.426	16.590	73.853	1.00	4.75	N
	ATOM 5919 CA METH 48	7.552	16.134	72.467	1.00	4.88	C
	ATOM 5920 C METH 48	8.335	14.829	72.376	1.00	7.28	C
	ATOM 5921 O METH 48	8.014	13.960	71.557	1.00	6.58	O
	ATOM 5922 CB METH 48	8.279	17.163	71.617	1.00	4.03	C
	ATOM 5923 CG METH 48	7.689	18.546	71.642	1.00	4.05	C
	ATOM 5924 SD METH 48	8.593	19.532	70.478	1.00	2.86	S
	ATOM 5925 CE METH 48	7.829	18.949	68.955	1.00	2.92	C
	ATOM 5926 N GLYH 40	0.306	14.724	73.175	1.00	8.01	N

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FIG. 53-92	ATOM 5928	C	GLY H 49	11.461	13.660	74.027	1.00	10.48	C
	ATOM 5929	O	GLY H 49	11.801	14.760	74.467	1.00	12.06	O
	ATOM 5930	N	ARG H 50	12.161	12.549	74.235	1.00	10.06	N
	ATOM 5931	CA	ARG H 50	13.365	12.547	75.058	1.00	9.26	C
	ATOM 5932	C	ARG H 50	14.386	11.544	74.569	1.00	9.54	C
	ATOM 5933	O	ARG H 50	14.031	10.419	74.229	1.00	12.18	O
	ATOM 5934	CB	ARG H 50	12.989	12.198	76.491	1.00	9.69	C
	ATOM 5935	CG	ARG H 50	14.156	11.905	77.402	1.00	9.78	C
	ATOM 5936	CD	ARG H 50	13.658	11.718	78.807	1.00	10.17	C
	ATOM 5937	NE	ARG H 50	14.697	11.207	79.689	1.00	13.80	N
	ATOM 5938	CZ	ARG H 50	14.762	9.950	80.118	1.00	13.53	C
	ATOM 5939	NH1	ARG H 50	13.849	9.067	79.729	1.00	12.57	N
	ATOM 5940	NH2	ARG H 50	15.696	9.596	80.995	1.00	14.85	N
	ATOM 5941	N	ILE H 51	15.655	11.932	74.564	1.00	8.81	N
	ATOM 5942	CA	ILE H 51	16.714	11.033	74.142	1.00	7.44	C
	ATOM 5943	C	ILE H 51	17.628	10.665	75.316	1.00	9.24	C
	ATOM 5944	O	ILE H 51	17.962	11.501	76.163	1.00	10.60	O
	ATOM 5945	CB	ILE H 51	17.536	11.601	72.941	1.00	5.75	C
	ATOM 5946	CG1	ILE H 51	18.647	10.621	72.547	1.00	3.54	C
	ATOM 5947	CG2	ILE H 51	18.060	12.995	73.243	1.00	4.92	C
	ATOM 5948	CD1	ILE H 51	19.577	11.116	71.468	1.00	2.00	C
	ATOM 5949	N	ILE H 52	17.942	9.375	75.399	1.00	9.98	N
	ATOM 5950	CA	ILE H 52	18.819	8.807	76.420	1.00	7.84	C
	ATOM 5951	C	ILE H 52	20.234	8.905	75.833	1.00	7.68	C
	ATOM 5952	O	ILE H 52	20.756	7.962	75.230	1.00	5.79	O
	ATOM 5953	CB	ILE H 52	18.410	7.324	76.701	1.00	6.65	C
	ATOM 5954	CG1	ILE H 52	16.951	7.267	77.174	1.00	4.76	C
	ATOM 5955	CG2	ILE H 52	19.343	6.679	77.718	1.00	4.82	C
	ATOM 5956	CD1	ILE H 52	16.406	5.865	77.394	1.00	3.25	C
	ATOM 5957	N	THR H 53	20.829	10.076	75.996	1.00	9.03	N
	ATOM 5958	CA	THR H 53	22.159	10.394	75.471	1.00	10.89	C
	ATOM 5959	C	THR H 53	23.320	9.376	75.572	1.00	12.64	C
	ATOM 5960	O	THR H 53	24.366	9.571	74.940	1.00	14.11	O
	ATOM 5961	CB	THR H 53	22.634	11.743	76.045	1.00	9.91	C
	ATOM 5962	OG1	THR H 53	21.492	12.583	76.290	1.00	9.80	O
	ATOM 5963	CG2	THR H 53	23.574	12.437	75.059	1.00	5.63	C
	ATOM 5964	N	ILE H 54	23.173	8.325	76.374	1.00	12.61	N
	ATOM 5965	CA	ILE H 54	24.239	7.326	76.507	1.00	12.19	C
	ATOM 5966	C	ILE H 54	24.081	6.241	75.429	1.00	12.10	C
	ATOM 5967	O	ILE H 54	25.050	5.831	74.795	1.00	10.19	O
	ATOM 5968	CB	ILE H 54	24.274	6.718	77.961	1.00	11.70	C
	ATOM 5969	CG1	ILE H 54	25.359	5.642	78.094	1.00	13.60	C
	ATOM 5970	CG2	ILE H 54	22.920	6.152	78.353	1.00	11.80	C
	ATOM 5971	CD1	ILE H 54	26.785	6.172	78.083	1.00	12.85	C
	ATOM 5972	N	LEU H 55	22.830	5.866	75.179	1.00	13.29	N
	ATOM 5973	CA	LEU H 55	22.435	4.847	74.200	1.00	12.91	C
	ATOM 5974	C	LEU H 55	22.031	5.402	72.831	1.00	14.22	C
	ATOM 5975	O	LEU H 55	22.029	4.664	71.843	1.00	16.37	O
	ATOM 5976	CB	LEU H 55	21.226	4.065	74.727	1.00	10.80	C
	ATOM 5977	CG	LEU H 55	21.307	2.919	75.729	1.00	9.21	C
	ATOM 5978	CD1	LEU H 55	22.658	2.893	76.415	1.00	10.96	C
	ATOM 5979	CD2	LEU H 55	20.158	3.047	76.719	1.00	5.46	C
	ATOM 5980	N	ASPH 56	21.617	6.665	72.793	1.00	15.31	N
	ATOM 5981	CA	ASPH 56	21.163	7.314	71.564	1.00	16.12	C
	ATOM 5982	C	ASPH 56	19.779	6.798	71.182	1.00	15.94	C
	ATOM 5983	O	ASPH 56	19.468	6.640	69.999	1.00	15.80	O
	ATOM 5984	CB	ASPH 56	22.132	7.088	70.405	1.00	18.24	C
	ATOM 5985	CG	ASPH 56	23.430	7.818	70.586	1.00	22.61	C
	ATOM 5986	OD1	ASPH 56	23.401	9.058	70.769	1.00	26.74	O
	ATOM 5987	OD2	ASPH 56	24.484	7.151	70.546	1.00	24.77	O
	ATOM 5988	N	VAL H 57	18.959	6.507	72.187	1.00	14.68	N
	ATOM 5989	CA	VAL H 57	17.610	6.012	71.936	1.00	13.55	C
	ATOM 5990	C	VAL H 57	16.605	7.019	72.450	1.00	12.46	C
	ATOM 5991	O	VAL H 57	16.552	7.297	73.647	1.00	11.82	O
	ATOM 5992	CB	VAL H 57	17.347	4.607	72.583	1.00	13.25	C
	ATOM 5993	CG1	VAL H 57	18.117	3.531	71.845	1.00	12.13	C
	ATOM 5994	CG2	VAL H 57	17.759	4.600	74.036	1.00	14.04	C
	ATOM 5995	N	ALAH 58	15.861	7.616	71.525	1.00	11.71	N
	ATOM 5996	CA	ALAH 58	14.847	8.603	71.873	1.00	10.71	C
	ATOM 5997	C	ALAH 58	12.466	7.068	71.821	1.00	10.16	C

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FIG. 53-93	ATOM 5999 CB ALA H 58	14.918	9.792	70.922	1.00	11.97	C
	ATOM 6000 N HISH 59	12.554	8.475	72.640	1.00	8.76	N
	ATOM 6001 CA HISH 59	11.190	7.973	72.720	1.00	9.14	C
	ATOM 6002 C HISH 59	10.303	9.201	72.578	1.00	12.02	C
	ATOM 6003 O HISH 59	10.303	10.074	73.455	1.00	14.15	O
	ATOM 6004 CB HISH 59	10.977	7.298	74.071	1.00	8.02	C
	ATOM 6005 CG HISH 59	11.842	6.099	74.276	1.00	7.40	C
	ATOM 6006 ND1 HISH 59	13.199	6.142	74.480	1.00	8.73	N
	ATOM 6007 CD2 HISH 59	11.522	4.776	74.260	1.00	7.19	C
	ATOM 6008 CE1 HISH 59	13.658	4.888	74.578	1.00	5.53	C
	ATOM 6009 NE2 HISH 59	12.674	4.022	74.449	1.00	5.46	N
	ATOM 6010 N TYR H 60	9.577	9.282	71.464	1.00	11.83	N
	ATOM 6011 CA TYR H 60	8.731	10.435	71.167	1.00	11.67	C
	ATOM 6012 C TYR H 60	7.289	10.281	71.577	1.00	11.43	C
	ATOM 6013 O TYR H 60	6.823	9.175	71.797	1.00	13.83	O
	ATOM 6014 CB TYR H 60	8.798	10.756	69.680	1.00	13.50	C
	ATOM 6015 CG TYR H 60	10.207	10.763	69.133	1.00	14.95	C
	ATOM 6016 CD1 TYR H 60	11.093	11.784	69.458	1.00	14.67	C
	ATOM 6017 CD2 TYR H 60	10.664	9.728	68.310	1.00	13.95	C
	ATOM 6018 CE1 TYR H 60	12.391	11.773	68.981	1.00	14.47	C
	ATOM 6019 CE2 TYR H 60	11.965	9.715	67.832	1.00	12.16	C
	ATOM 6020 CZ TYR H 60	12.819	10.738	68.172	1.00	12.33	C
	ATOM 6021 OH TYR H 60	14.107	10.739	67.704	1.00	13.46	O
	ATOM 6022 N ALA H 61	6.583	11.403	71.633	1.00	11.41	N
	ATOM 6023 CA ALA H 61	5.181	11.434	72.026	1.00	13.02	C
	ATOM 6024 C ALA H 61	4.270	10.905	70.911	1.00	14.85	C
	ATOM 6025 O ALA H 61	4.409	11.277	69.745	1.00	16.00	O
	ATOM 6026 CB ALA H 61	4.782	12.857	72.404	1.00	11.91	C
	ATOM 6027 N PRO H 62	3.305	10.046	71.261	1.00	15.17	N
	ATOM 6028 CA PRO H 62	2.386	9.485	70.271	1.00	15.38	C
	ATOM 6029 C PRO H 62	1.406	10.499	69.650	1.00	17.18	C
	ATOM 6030 O PRO H 62	0.206	10.502	69.956	1.00	19.60	O
	ATOM 6031 CB PRO H 62	1.683	8.386	71.061	1.00	14.73	C
	ATOM 6032 CG PRO H 62	1.692	8.924	72.459	1.00	16.02	C
	ATOM 6033 CD PRO H 62	3.078	9.451	72.589	1.00	15.20	C
	ATOM 6034 N HISH 63	1.943	11.359	68.788	1.00	16.39	N
	ATOM 6035 CA HISH 63	1.195	12.387	68.060	1.00	15.11	C
	ATOM 6036 C HISH 63	2.208	13.130	67.189	1.00	14.22	C
	ATOM 6037 O HISH 63	1.865	13.741	66.181	1.00	13.83	O
	ATOM 6038 CB HISH 63	0.416	13.338	69.002	1.00	14.89	C
	ATOM 6039 CG HISH 63	1.216	14.480	69.565	1.00	15.15	C
	ATOM 6040 ND1 HISH 63	1.762	14.455	70.831	1.00	15.98	N
	ATOM 6041 CD2 HISH 63	1.480	15.713	69.071	1.00	13.13	C
	ATOM 6042 CE1 HISH 63	2.327	15.621	71.095	1.00	12.59	C
	ATOM 6043 NE2 HISH 63	2.169	16.401	70.043	1.00	13.03	N
	ATOM 6044 N LEU H 64	3.465	13.067	67.611	1.00	13.05	N
	ATOM 6045 CA LEU H 64	4.582	13.684	66.913	1.00	12.91	C
	ATOM 6046 C LEU H 64	5.381	12.577	66.233	1.00	14.95	C
	ATOM 6047 O LEU H 64	6.140	12.827	65.294	1.00	16.52	O
	ATOM 6048 CB LEU H 64	5.474	14.400	67.926	1.00	12.13	C
	ATOM 6049 CG LEU H 64	5.459	15.928	67.970	1.00	9.82	C
	ATOM 6050 CD1 LEU H 64	4.109	16.479	67.568	1.00	10.49	C
	ATOM 6051 CD2 LEU H 64	5.821	16.377	69.346	1.00	6.56	C
	ATOM 6052 N GLN H 65	5.218	11.357	66.747	1.00	16.31	N
	ATOM 6053 CA GLN H 65	5.896	10.171	66.233	1.00	15.36	C
	ATOM 6054 C GLN H 65	5.728	10.090	64.721	1.00	13.38	C
	ATOM 6055 O GLN H 65	4.608	10.124	64.198	1.00	11.85	O
	ATOM 6056 CB GLN H 65	5.337	8.908	66.909	1.00	16.10	C
	ATOM 6057 CG GLN H 65	5.923	7.570	66.411	1.00	17.28	C
	ATOM 6058 CD GLN H 65	7.381	7.347	66.814	1.00	17.41	C
	ATOM 6059 OE1 GLN H 65	8.224	7.026	65.981	1.00	16.73	O
	ATOM 6060 NE2 GLN H 65	7.674	7.494	68.096	1.00	18.80	N
	ATOM 6061 N GLY H 66	6.857	10.010	64.034	1.00	11.47	N
	ATOM 6062 CA GLY H 66	6.844	9.935	62.595	1.00	12.23	C
	ATOM 6063 C GLY H 66	7.432	11.182	61.969	1.00	12.71	C
	ATOM 6064 O GLY H 66	8.208	11.087	61.007	1.00	13.79	O
	ATOM 6065 N ARG H 67	7.103	12.349	62.526	1.00	12.38	N
	ATOM 6066 CA ARG H 67	7.597	13.616	61.984	1.00	11.52	C
	ATOM 6067 C ARG H 67	8.486	14.424	62.917	1.00	10.81	C
	ATOM 6068 O ARG H 67	8.722	15.500	62.691	1.00	12.22	O

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FIG. 53-94

ATOM 6070	CG ARGH 67	5.580	14.954	62.680	1.00	11.31	C
ATOM 6071	CD ARGH 67	4.372	15.659	62.146	1.00	11.22	C
ATOM 6072	NE ARGH 67	3.681	16.411	63.183	1.00	12.42	N
ATOM 6073	CZ ARGH 67	3.766	17.725	63.311	1.00	11.37	C
ATOM 6074	NH1 ARGH 67	4.518	18.420	62.470	1.00	13.94	N
ATOM 6075	NH2 ARGH 67	3.065	18.348	64.238	1.00	11.68	N
ATOM 6076	N VALH 68	8.979	13.790	63.966	1.00	10.98	N
ATOM 6077	CA VALH 68	9.850	14.455	64.926	1.00	8.54	C
ATOM 6078	C VALH 68	11.088	13.585	65.116	1.00	8.61	C
ATOM 6079	O VALH 68	10.988	12.357	65.122	1.00	9.69	O
ATOM 6080	CB VALH 68	9.145	14.626	66.266	1.00	4.87	C
ATOM 6081	CG1 VALH 68	8.779	13.279	66.823	1.00	3.96	C
ATOM 6082	CG2 VALH 68	10.031	15.385	67.213	1.00	2.00	C
ATOM 6083	N THRH 69	12.245	14.209	65.291	1.00	7.97	N
ATOM 6084	CA THRH 69	13.482	13.465	65.458	1.00	7.36	C
ATOM 6085	C THRH 69	14.488	14.174	66.356	1.00	7.00	C
ATOM 6086	O THRH 69	14.910	15.297	66.076	1.00	6.55	O
ATOM 6087	CB THRH 69	14.135	13.212	64.086	1.00	9.59	C
ATOM 6088	OG1 THRH 69	13.221	12.481	63.250	1.00	9.97	O
ATOM 6089	CG2 THRH 69	15.453	12.447	64.238	1.00	7.33	C
ATOM 6090	N ILEH 70	14.906	13.499	67.418	1.00	7.70	N
ATOM 6091	CA ILEH 70	15.882	14.084	68.330	1.00	8.61	C
ATOM 6092	C ILEH 70	17.187	13.297	68.226	1.00	8.12	C
ATOM 6093	O ILEH 70	17.174	12.079	68.104	1.00	7.33	O
ATOM 6094	CB ILEH 70	15.373	14.081	69.806	1.00	7.10	C
ATOM 6095	CG1 ILEH 70	13.936	14.606	69.872	1.00	6.03	C
ATOM 6096	CG2 ILEH 70	16.260	14.965	70.664	1.00	4.82	C
ATOM 6097	CD1 ILEH 70	13.321	14.525	71.249	1.00	6.55	C
ATOM 6098	N THRH 71	18.301	14.016	68.188	1.00	9.35	N
ATOM 6099	CA THRH 71	19.626	13.410	68.111	1.00	9.64	C
ATOM 6100	C THRH 71	20.553	14.239	68.968	1.00	11.13	C
ATOM 6101	O THRH 71	20.283	15.414	69.223	1.00	12.66	O
ATOM 6102	CB THRH 71	20.199	13.389	66.666	1.00	9.37	C
ATOM 6103	OG1 THRH 71	20.079	14.688	66.072	1.00	7.60	O
ATOM 6104	CG2 THRH 71	19.494	12.343	65.807	1.00	8.15	C
ATOM 6105	N ALAH 72	21.626	13.621	69.440	1.00	12.83	N
ATOM 6106	CA ALAH 72	22.597	14.315	70.259	1.00	14.33	C
ATOM 6107	C ALAH 72	23.951	13.964	69.695	1.00	16.43	C
ATOM 6108	O ALAH 72	24.210	12.807	69.384	1.00	16.79	O
ATOM 6109	CB ALAH 72	22.493	13.871	71.700	1.00	14.21	C
ATOM 6110	N ASPH 73	24.752	14.981	69.410	1.00	19.82	N
ATOM 6111	CA ASPH 73	26.088	14.754	68.905	1.00	21.26	C
ATOM 6112	C ASPH 73	26.945	14.764	70.158	1.00	21.75	C
ATOM 6113	O ASPH 73	27.011	15.764	70.874	1.00	21.34	O
ATOM 6114	CB ASPH 73	26.512	15.862	67.936	1.00	21.84	C
ATOM 6115	CG ASPH 73	27.880	15.604	67.305	1.00	24.12	C
ATOM 6116	OD1 ASPH 73	28.662	14.782	67.823	1.00	24.23	O
ATOM 6117	OD2 ASPH 73	28.191	16.242	66.282	1.00	27.83	O
ATOM 6118	N LYSH 74	27.555	13.626	70.453	1.00	23.06	N
ATOM 6119	CA LYSH 74	28.386	13.500	71.635	1.00	25.10	C
ATOM 6120	C LYSH 74	29.732	14.223	71.520	1.00	26.71	C
ATOM 6121	O LYSH 74	30.392	14.461	72.535	1.00	28.49	O
ATOM 6122	CB LYSH 74	28.574	12.020	71.982	1.00	25.76	C
ATOM 6123	CG LYSH 74	28.442	11.718	73.470	1.00	26.80	C
ATOM 6124	CD LYSH 74	29.699	12.112	74.215	1.00	28.23	C
ATOM 6125	CE LYSH 74	29.376	12.712	75.568	1.00	27.87	C
ATOM 6126	NZ LYSH 74	30.622	13.097	76.280	1.00	25.28	N
ATOM 6127	N SERH 75	30.131	14.591	70.304	1.00	26.51	N
ATOM 6128	CA SERH 75	31.396	15.301	70.111	1.00	27.08	C
ATOM 6129	C SERH 75	31.239	16.817	70.237	1.00	26.42	C
ATOM 6130	O SERH 75	32.218	17.523	70.429	1.00	27.72	O
ATOM 6131	CB SERH 75	32.031	14.964	68.756	1.00	28.79	C
ATOM 6132	OG SERH 75	31.455	15.726	67.703	1.00	30.42	O
ATOM 6133	N THRH 76	30.023	17.328	70.087	1.00	25.32	N
ATOM 6134	CA THRH 76	29.804	18.765	70.207	1.00	25.03	C
ATOM 6135	C THRH 76	28.834	19.066	71.348	1.00	26.48	C
ATOM 6136	O THRH 76	28.349	20.197	71.482	1.00	28.52	O
ATOM 6137	CB THRH 76	29.230	19.374	68.900	1.00	24.27	C
ATOM 6138	OG1 THRH 76	28.024	18.691	68.536	1.00	23.85	O
ATOM 6139	CG2 THRH 76	20.220	10.278	67.762	1.00	25.04	C

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FIG. 53-95	ATOM 6141	CA SER H 77	27.608	18.209	73.278	1.00	23.20	C
	ATOM 6142	C SER H 77	26.383	18.961	72.789	1.00	21.34	C
	ATOM 6143	O SER H 77	25.941	19.925	73.410	1.00	21.95	O
	ATOM 6144	CB SER H 77	28.260	18.957	74.440	1.00	22.09	C
	ATOM 6145	OG SER H 77	29.178	18.130	75.133	1.00	23.49	O
	ATOM 6146	N THR H 78	25.839	18.523	71.666	1.00	18.26	N
	ATOM 6147	CA THR H 78	24.691	19.206	71.115	1.00	17.69	C
	ATOM 6148	C THR H 78	23.495	18.309	70.868	1.00	15.95	C
	ATOM 6149	O THR H 78	23.613	17.251	70.242	1.00	16.03	O
	ATOM 6150	CB THR H 78	25.063	19.913	69.800	1.00	19.01	C
	ATOM 6151	OG1 THR H 78	26.186	20.773	70.031	1.00	19.55	O
	ATOM 6152	CG2 THR H 78	23.887	20.744	69.285	1.00	16.29	C
	ATOM 6153	N VAL H 79	22.349	18.728	71.386	1.00	12.40	N
	ATOM 6154	CA VAL H 79	21.111	17.997	71.187	1.00	9.30	C
	ATOM 6155	C VAL H 79	20.452	18.627	69.956	1.00	7.84	C
	ATOM 6156	O VAL H 79	20.746	19.782	69.609	1.00	6.59	O
	ATOM 6157	CB VAL H 79	20.202	18.142	72.411	1.00	10.45	C
	ATOM 6158	CG1 VAL H 79	18.923	17.318	72.238	1.00	8.32	C
	ATOM 6159	CG2 VAL H 79	20.967	17.723	73.664	1.00	10.05	C
	ATOM 6160	N TYR H 80	19.580	17.882	69.287	1.00	5.53	N
	ATOM 6161	CA TYR H 80	18.913	18.391	68.091	1.00	4.33	C
	ATOM 6162	C TYR H 80	17.461	17.987	68.072	1.00	3.56	C
	ATOM 6163	O TYR H 80	17.088	16.997	68.694	1.00	7.00	O
	ATOM 6164	CB TYR H 80	19.573	17.835	66.822	1.00	2.98	C
	ATOM 6165	CG TYR H 80	20.886	18.477	66.468	1.00	3.35	C
	ATOM 6166	CD1 TYR H 80	20.925	19.665	65.745	1.00	3.20	C
	ATOM 6167	CD2 TYR H 80	22.092	17.913	66.876	1.00	3.31	C
	ATOM 6168	CE1 TYR H 80	22.133	20.280	65.447	1.00	5.35	C
	ATOM 6169	CE2 TYR H 80	23.302	18.518	66.582	1.00	4.91	C
	ATOM 6170	CZ TYR H 80	23.318	19.700	65.871	1.00	5.18	C
	ATOM 6171	OH TYR H 80	24.518	20.321	65.623	1.00	6.56	O
	ATOM 6172	N LEU H 81	16.651	18.743	67.340	1.00	2.64	N
	ATOM 6173	CA LEU H 81	15.241	18.435	67.187	1.00	3.48	C
	ATOM 6174	C LEU H 81	14.854	18.843	65.784	1.00	5.71	C
	ATOM 6175	O LEU H 81	14.997	20.012	65.415	1.00	7.81	O
	ATOM 6176	CB LEU H 81	14.387	19.202	68.194	1.00	2.00	C
	ATOM 6177	CG LEU H 81	12.891	18.890	68.410	1.00	3.11	C
	ATOM 6178	CD1 LEU H 81	12.050	20.133	68.146	1.00	2.00	C
	ATOM 6179	CD2 LEU H 81	12.396	17.710	67.607	1.00	2.00	C
	ATOM 6180	N GLU H 82	14.497	17.864	64.960	1.00	7.38	N
	ATOM 6181	CA GLU H 82	14.051	18.172	63.614	1.00	10.06	C
	ATOM 6182	C GLU H 82	12.577	17.895	63.614	1.00	9.49	C
	ATOM 6183	O GLU H 82	12.145	16.879	64.139	1.00	9.65	O
	ATOM 6184	CB GLU H 82	14.703	17.316	62.529	1.00	10.92	C
	ATOM 6185	CG GLU H 82	14.310	17.832	61.144	1.00	14.26	C
	ATOM 6186	CD GLU H 82	14.779	16.966	60.008	1.00	18.22	C
	ATOM 6187	OE1 GLU H 82	15.929	17.160	59.551	1.00	20.46	O
	ATOM 6188	OE2 GLU H 82	13.987	16.103	59.556	1.00	21.67	O
	ATOM 6189	N LEU H 83	11.809	18.807	63.047	1.00	9.97	N
	ATOM 6190	CA LEU H 83	10.373	18.647	62.980	1.00	10.94	C
	ATOM 6191	C LEU H 83	10.020	18.862	61.515	1.00	12.02	C
	ATOM 6192	O LEU H 83	10.289	19.925	60.941	1.00	12.61	O
	ATOM 6193	CB LEU H 83	9.679	19.659	63.906	1.00	8.22	C
	ATOM 6194	CG LEU H 83	8.282	19.331	64.438	1.00	3.41	C
	ATOM 6195	CD1 LEU H 83	7.239	19.664	63.423	1.00	4.50	C
	ATOM 6196	CD2 LEU H 83	8.206	17.876	64.798	1.00	2.00	C
	ATOM 6197	N ARG H 84	9.515	17.806	60.885	1.00	12.66	N
	ATOM 6198	CA ARG H 84	9.171	17.869	59.482	1.00	12.67	C
	ATOM 6199	C ARG H 84	7.675	17.981	59.275	1.00	13.55	C
	ATOM 6200	O ARG H 84	6.895	17.817	60.216	1.00	13.09	O
	ATOM 6201	CB ARG H 84	9.756	16.664	58.743	1.00	13.20	C
	ATOM 6202	CG ARG H 84	9.181	15.329	59.178	1.00	15.41	C
	ATOM 6203	CD ARG H 84	10.118	14.207	58.780	1.00	13.44	C
	ATOM 6204	NE ARG H 84	11.392	14.347	59.483	1.00	10.62	N
	ATOM 6205	CZ ARG H 84	11.758	13.614	60.529	1.00	6.51	C
	ATOM 6206	NH1 ARG H 84	10.950	12.664	61.005	1.00	3.06	N
	ATOM 6207	NH2 ARG H 84	12.921	13.870	61.115	1.00	2.00	N
	ATOM 6208	N ASN H 85	7.292	18.278	58.035	1.00	14.44	N
	ATOM 6209	CA ASN H 85	5.901	18.462	57.656	1.00	15.43	C
	ATOM 6210	C ASN H 85	5.270	18.546	58.536	1.00	16.34	C



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FIG. 53-96	ATOM 6212	CB ASNH 85	5.132	17.143	57.732	1.00	17.57	C
	ATOM 6213	CG ASNH 85	5.594	16.141	56.681	1.00	18.99	C
	ATOM 6214	OD1 ASNH 85	5.725	14.944	56.952	1.00	17.64	O
	ATOM 6215	ND2 ASNH 85	5.854	16.631	55.476	1.00	18.85	N
	ATOM 6216	N LEUH 86	6.010	20.651	58.663	1.00	16.01	N
	ATOM 6217	CA LEUH 86	5.559	21.769	59.471	1.00	16.50	C
	ATOM 6218	C LEUH 86	4.161	22.225	59.124	1.00	17.21	C
	ATOM 6219	O LEUH 86	3.823	22.425	57.950	1.00	18.15	O
	ATOM 6220	CB LEUH 86	6.524	22.947	59.375	1.00	14.51	C
	ATOM 6221	CG LEUH 86	7.736	22.824	60.297	1.00	14.88	C
	ATOM 6222	CD1 LEUH 86	8.742	23.907	59.985	1.00	14.47	C
	ATOM 6223	CD2 LEUH 86	7.300	22.896	61.750	1.00	13.40	C
	ATOM 6224	N ARGH 87	3.324	22.262	60.152	1.00	17.78	N
	ATOM 6225	CA ARGH 87	1.947	22.715	60.049	1.00	15.84	C
	ATOM 6226	C ARGH 87	1.994	24.080	60.733	1.00	13.95	C
	ATOM 6227	O ARGH 87	2.875	24.334	61.560	1.00	11.95	O
	ATOM 6228	CB ARGH 87	1.026	21.761	60.821	1.00	17.40	C
	ATOM 6229	CG ARGH 87	0.758	20.438	60.123	1.00	21.87	C
	ATOM 6230	CD ARGH 87	-0.359	20.572	59.089	1.00	26.43	C
	ATOM 6231	NE ARGH 87	-0.135	19.781	57.874	1.00	31.72	N
	ATOM 6232	CZ ARGH 87	0.788	20.057	56.946	1.00	32.88	C
	ATOM 6233	NH1 ARGH 87	1.588	21.114	57.086	1.00	33.85	N
	ATOM 6234	NH2 ARGH 87	0.922	19.267	55.885	1.00	32.25	N
	ATOM 6235	N SERH 88	1.074	24.968	60.387	1.00	13.21	N
	ATOM 6236	CA SERH 88	1.070	26.279	61.007	1.00	14.50	C
	ATOM 6237	C SERH 88	0.905	26.139	62.522	1.00	14.12	C
	ATOM 6238	O SERH 88	1.407	26.963	63.294	1.00	14.71	O
	ATOM 6239	CB SERH 88	-0.029	27.164	60.409	1.00	14.65	C
	ATOM 6240	OG SERH 88	-1.321	26.691	60.735	1.00	16.47	O
	ATOM 6241	N ASPH 89	0.250	25.068	62.956	1.00	13.49	N
	ATOM 6242	CA ASPH 89	0.049	24.857	64.384	1.00	12.51	C
	ATOM 6243	C ASPH 89	1.309	24.452	65.138	1.00	11.36	C
	ATOM 6244	O ASPH 89	1.308	24.407	66.369	1.00	12.92	O
	ATOM 6245	CB ASPH 89	-1.090	23.876	64.644	1.00	12.20	C
	ATOM 6246	CG ASPH 89	-0.900	22.576	63.947	1.00	10.88	C
	ATOM 6247	OD1 ASPH 89	-1.299	22.485	62.765	1.00	10.68	O
	ATOM 6248	OD2 ASPH 89	-0.359	21.651	64.581	1.00	7.76	O
	ATOM 6249	N ASPH 90	2.395	24.202	64.414	1.00	10.72	N
	ATOM 6250	CA ASPH 90	3.653	23.847	65.057	1.00	10.33	C
	ATOM 6251	C ASPH 90	4.378	25.114	65.527	1.00	10.46	C
	ATOM 6252	O ASPH 90	5.488	25.043	66.053	1.00	11.49	O
	ATOM 6253	CB ASPH 90	4.549	23.027	64.118	1.00	10.98	C
	ATOM 6254	CG ASPH 90	4.062	21.573	63.931	1.00	12.18	C
	ATOM 6255	OD1 ASPH 90	3.655	20.904	64.910	1.00	7.09	O
	ATOM 6256	OD2 ASPH 90	4.104	21.076	62.785	1.00	14.56	O
	ATOM 6257	N THR H 91	3.750	26.272	65.319	1.00	10.54	N
	ATOM 6258	CA THR H 91	4.299	27.569	65.725	1.00	9.98	C
	ATOM 6259	C THR H 91	4.365	27.650	67.251	1.00	9.59	C
	ATOM 6260	O THR H 91	3.334	27.785	67.924	1.00	8.95	O
	ATOM 6261	CB THR H 91	3.414	28.730	65.238	1.00	10.45	C
	ATOM 6262	OG1 THR H 91	3.290	28.696	63.811	1.00	12.36	O
	ATOM 6263	CG2 THR H 91	4.030	30.053	65.637	1.00	12.42	C
	ATOM 6264	N ALAH 92	5.573	27.611	67.795	1.00	9.83	N
	ATOM 6265	CA ALAH 92	5.729	27.654	69.233	1.00	9.74	C
	ATOM 6266	C ALAH 92	7.170	27.879	69.619	1.00	9.44	C
	ATOM 6267	O ALAH 92	8.038	28.029	68.763	1.00	11.18	O
	ATOM 6268	CB ALAH 92	5.242	26.355	69.833	1.00	12.61	C
	ATOM 6269	N VALH 93	7.414	27.898	70.922	1.00	8.45	N
	ATOM 6270	CA VALH 93	8.747	28.094	71.469	1.00	6.72	C
	ATOM 6271	C VALH 93	9.235	26.723	71.924	1.00	7.96	C
	ATOM 6272	O VALH 93	8.584	26.053	72.728	1.00	7.93	O
	ATOM 6273	CB VALH 93	8.710	29.040	72.658	1.00	3.48	C
	ATOM 6274	CG1 VALH 93	10.101	29.382	73.094	1.00	4.97	C
	ATOM 6275	CG2 VALH 93	7.954	30.286	72.300	1.00	2.20	C
	ATOM 6276	N TYRH 94	10.373	26.309	71.379	1.00	8.12	N
	ATOM 6277	CA TYRH 94	10.956	25.013	71.674	1.00	7.75	C
	ATOM 6278	C TYRH 94	12.116	25.055	72.665	1.00	6.30	C
	ATOM 6279	O TYRH 94	13.185	25.602	72.370	1.00	2.95	O
	ATOM 6280	CB TYRH 94	11.385	24.340	70.361	1.00	11.44	C

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FIG. 53-97

ATOM 6283	CD2 TYR H 94	10.127	22.750	68.829	1.00	14.37	C
ATOM 6284	CE1 TYR H 94	8.045	24.561	68.499	1.00	16.79	C
ATOM 6285	CE2 TYR H 94	9.013	22.408	68.049	1.00	14.35	C
ATOM 6286	CZ TYR H 94	7.972	23.315	67.898	1.00	14.14	C
ATOM 6287	OH TYR H 94	6.827	22.958	67.221	1.00	11.38	O
ATOM 6288	N PHE H 95	11.881	24.502	73.853	1.00	6.46	N
ATOM 6289	CA PHE H 95	12.901	24.441	74.894	1.00	6.88	C
ATOM 6290	C PHE H 95	13.543	23.067	74.917	1.00	7.73	C
ATOM 6291	O PHE H 95	12.877	22.065	74.644	1.00	6.89	O
ATOM 6292	CB PHE H 95	12.291	24.626	76.284	1.00	4.64	C
ATOM 6293	CG PHE H 95	11.514	25.884	76.453	1.00	4.70	C
ATOM 6294	CD1 PHE H 95	12.167	27.095	76.684	1.00	4.65	C
ATOM 6295	CD2 PHE H 95	10.130	25.861	76.430	1.00	2.33	C
ATOM 6296	CE1 PHE H 95	11.456	28.253	76.891	1.00	2.34	C
ATOM 6297	CE2 PHE H 95	9.408	27.020	76.637	1.00	4.85	C
ATOM 6298	CZ PHE H 95	10.076	28.225	76.870	1.00	3.13	C
ATOM 6299	N CYSH 96	14.835	23.024	75.214	1.00	8.72	N
ATOM 6300	CA CYSH 96	15.523	21.757	75.382	1.00	10.25	C
ATOM 6301	C CYSH 96	15.733	21.734	76.894	1.00	10.64	C
ATOM 6302	O CYSH 96	15.935	22.790	77.513	1.00	11.69	O
ATOM 6303	CB CYSH 96	16.865	21.720	74.640	1.00	11.55	C
ATOM 6304	SG CYSH 96	18.050	23.018	75.110	1.00	17.70	S
ATOM 6305	N ALA H 97	15.621	20.566	77.510	1.00	9.40	N
ATOM 6306	CA ALA H 97	15.806	20.475	78.954	1.00	7.79	C
ATOM 6307	C ALA H 97	16.595	19.227	79.279	1.00	7.44	C
ATOM 6308	O ALA H 97	16.989	18.494	78.384	1.00	8.41	O
ATOM 6309	CB ALA H 97	14.459	20.451	79.653	1.00	7.01	C
ATOM 6310	N GLY H 98	16.837	18.990	80.558	1.00	8.12	N
ATOM 6311	CA GLY H 98	17.578	17.811	80.946	1.00	7.91	C
ATOM 6312	C GLY H 98	17.827	17.679	82.427	1.00	7.80	C
ATOM 6313	O GLY H 98	17.630	18.621	83.202	1.00	7.39	O
ATOM 6314	N VAL H 99	18.168	16.457	82.823	1.00	9.74	N
ATOM 6315	CA VAL H 99	18.501	16.113	84.201	1.00	11.02	C
ATOM 6316	C VAL H 99	19.730	15.240	84.106	1.00	11.60	C
ATOM 6317	O VAL H 99	20.126	14.821	83.022	1.00	13.99	O
ATOM 6318	CB VAL H 99	17.412	15.290	84.919	1.00	10.75	C
ATOM 6319	CG1 VAL H 99	16.259	16.173	85.304	1.00	11.64	C
ATOM 6320	CG2 VAL H 99	16.948	14.135	84.040	1.00	13.26	C
ATOM 6321	N TYR H 100	20.325	14.957	85.249	1.00	11.05	N
ATOM 6322	CA TYR H 100	21.518	14.138	85.318	1.00	7.98	C
ATOM 6323	C TYR H 100	21.123	12.763	85.824	1.00	6.09	C
ATOM 6324	O TYR H 100	20.302	12.654	86.737	1.00	4.87	O
ATOM 6325	CB TYR H 100	22.515	14.817	86.256	1.00	7.21	C
ATOM 6326	CG TYR H 100	23.632	13.960	86.746	1.00	3.12	C
ATOM 6327	CD1 TYR H 100	23.466	13.151	87.861	1.00	2.00	C
ATOM 6328	CD2 TYR H 100	24.868	13.988	86.123	1.00	3.75	C
ATOM 6329	CE1 TYR H 100	24.498	12.396	88.344	1.00	2.00	C
ATOM 6330	CE2 TYR H 100	25.923	13.224	86.600	1.00	4.79	C
ATOM 6331	CZ TYR H 100	25.731	12.433	87.716	1.00	2.60	C
ATOM 6332	OH TYR H 100	26.779	11.707	88.207	1.00	4.31	O
ATOM 6333	N GLU H 101	21.690	11.736	85.194	1.00	6.38	N
ATOM 6334	CA GLU H 101	21.441	10.328	85.519	1.00	6.30	C
ATOM 6335	C GLU H 101	22.628	9.741	86.301	1.00	7.29	C
ATOM 6336	O GLU H 101	22.465	9.282	87.423	1.00	6.15	O
ATOM 6337	CB GLU H 101	21.221	9.531	84.223	1.00	5.89	C
ATOM 6338	CG GLU H 101	20.277	10.174	83.187	1.00	3.98	C
ATOM 6339	CD GLU H 101	18.800	10.099	83.563	1.00	5.47	C
ATOM 6340	OE1 GLU H 101	18.494	9.684	84.697	1.00	7.08	O
ATOM 6341	OE2 GLU H 101	17.929	10.455	82.733	1.00	2.69	O
ATOM 6342	N GLY H 102	23.821	9.752	85.706	1.00	9.60	N
ATOM 6343	CA GLY H 102	24.995	9.237	86.395	1.00	12.31	C
ATOM 6344	C GLY H 102	25.905	8.258	85.666	1.00	16.39	C
ATOM 6345	O GLY H 102	26.983	7.950	86.165	1.00	15.66	O
ATOM 6346	N GLU H 103	25.496	7.817	84.479	1.00	20.62	N
ATOM 6347	CA GLU H 103	26.242	6.845	83.673	1.00	24.85	C
ATOM 6348	C GLU H 103	27.737	7.113	83.447	1.00	27.34	C
ATOM 6349	O GLU H 103	28.505	7.076	84.399	1.00	30.02	O
ATOM 6350	CB GLU H 103	25.477	6.583	82.367	1.00	26.05	C
ATOM 6351	CG GLU H 103	26.151	5.678	81.326	1.00	30.53	C
ATOM 6352	CD GLU H 103	26.767	4.408	81.883	1.00	31.41	C

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FIG. 53-98	ATOM 6354	OE2 GLU H 103	26.113	3.348	81.832	1.00	33.96	O
	ATOM 6355	N ALA H 104	28.159	7.362	82.209	1.00	29.27	N
	ATOM 6356	CA ALA H 104	29.570	7.599	81.886	1.00	30.55	C
	ATOM 6357	C ALA H 104	30.494	6.499	82.400	1.00	30.87	C
	ATOM 6358	O ALA H 104	31.388	6.757	83.213	1.00	30.76	O
	ATOM 6359	CB ALA H 104	30.025	8.954	82.407	1.00	30.95	C
	ATOM 6360	N ASP H 105	30.291	5.291	81.881	1.00	32.13	N
	ATOM 6361	CA ASP H 105	31.063	4.104	82.241	1.00	33.17	C
	ATOM 6362	C ASP H 105	31.007	3.834	83.736	1.00	33.82	C
	ATOM 6363	O ASP H 105	32.013	3.875	84.455	1.00	36.41	O
	ATOM 6364	CB ASP H 105	32.508	4.184	81.730	1.00	34.46	C
	ATOM 6365	CG ASP H 105	32.600	4.150	80.203	1.00	36.30	C
	ATOM 6366	OD1 ASP H 105	31.555	4.016	79.521	1.00	36.30	O
	ATOM 6367	OD2 ASP H 105	33.726	4.281	79.676	1.00	36.00	O
	ATOM 6368	N GLU H 106	29.788	3.602	84.197	1.00	31.59	N
	ATOM 6369	CA GLU H 106	29.494	3.287	85.585	1.00	27.78	C
	ATOM 6370	C GLU H 106	28.275	2.369	85.548	1.00	25.32	C
	ATOM 6371	O GLU H 106	28.024	1.627	86.499	1.00	26.26	O
	ATOM 6372	CB GLU H 106	29.161	4.549	86.383	1.00	27.49	C
	ATOM 6373	CG GLU H 106	30.310	5.517	86.575	1.00	27.59	C
	ATOM 6374	CD GLU H 106	29.980	6.606	87.582	1.00	27.57	C
	ATOM 6375	OE1 GLU H 106	29.898	6.304	88.790	1.00	28.56	O
	ATOM 6376	OE2 GLU H 106	29.817	7.767	87.185	1.00	24.49	O
	ATOM 6377	N GLY H 107	27.521	2.438	84.451	1.00	21.84	N
	ATOM 6378	CA GLY H 107	26.343	1.613	84.275	1.00	18.93	C
	ATOM 6379	C GLY H 107	25.117	2.132	84.991	1.00	18.22	C
	ATOM 6380	O GLY H 107	24.013	1.655	84.735	1.00	17.35	O
	ATOM 6381	N GLU H 108	25.311	3.087	85.901	1.00	18.06	N
	ATOM 6382	CA GLU H 108	24.218	3.674	86.681	1.00	16.77	C
	ATOM 6383	C GLU H 108	23.404	4.632	85.816	1.00	15.01	C
	ATOM 6384	O GLU H 108	23.962	5.403	85.041	1.00	15.22	O
	ATOM 6385	CB GLU H 108	24.778	4.403	87.901	1.00	17.99	C
	ATOM 6386	CG GLU H 108	23.715	4.903	88.859	1.00	19.84	C
	ATOM 6387	CD GLU H 108	24.290	5.769	89.948	1.00	20.33	C
	ATOM 6388	OE1 GLU H 108	24.510	6.964	89.685	1.00	22.12	O
	ATOM 6389	OE2 GLU H 108	24.545	5.262	91.062	1.00	20.70	O
	ATOM 6390	N TYR H 109	22.090	4.612	85.981	1.00	13.44	N
	ATOM 6391	CA TYR H 109	21.216	5.438	85.170	1.00	13.22	C
	ATOM 6392	C TYR H 109	19.809	5.411	85.753	1.00	13.74	C
	ATOM 6393	O TYR H 109	19.050	4.471	85.510	1.00	14.84	O
	ATOM 6394	CB TYR H 109	21.198	4.877	83.745	1.00	13.35	C
	ATOM 6395	CG TYR H 109	20.833	5.877	82.692	1.00	13.43	C
	ATOM 6396	CD1 TYR H 109	21.780	6.772	82.204	1.00	15.22	C
	ATOM 6397	CD2 TYR H 109	19.528	5.976	82.223	1.00	14.92	C
	ATOM 6398	CE1 TYR H 109	21.433	7.753	81.275	1.00	15.72	C
	ATOM 6399	CE2 TYR H 109	19.170	6.950	81.296	1.00	15.14	C
	ATOM 6400	CZ TYR H 109	20.127	7.837	80.833	1.00	15.74	C
	ATOM 6401	OH TYR H 109	19.764	8.826	79.955	1.00	18.81	O
	ATOM 6402	N ASP H 110	19.461	6.455	86.499	1.00	14.02	N
	ATOM 6403	CA ASP H 110	18.150	6.568	87.141	1.00	14.21	C
	ATOM 6404	C ASP H 110	16.998	6.584	86.153	1.00	12.92	C
	ATOM 6405	O ASP H 110	15.931	6.034	86.421	1.00	12.58	O
	ATOM 6406	CB ASP H 110	18.058	7.871	87.948	1.00	17.79	C
	ATOM 6407	CG ASP H 110	18.872	7.852	89.221	1.00	23.07	C
	ATOM 6408	OD1 ASP H 110	19.909	7.160	89.272	1.00	26.33	O
	ATOM 6409	OD2 ASP H 110	18.481	8.567	90.173	1.00	25.02	O
	ATOM 6410	N ASN H 111	17.222	7.267	85.031	1.00	12.61	N
	ATOM 6411	CA ASN H 111	16.232	7.479	83.978	1.00	10.59	C
	ATOM 6412	C ASN H 111	15.194	8.448	84.542	1.00	9.97	C
	ATOM 6413	O ASN H 111	13.989	8.220	84.436	1.00	10.86	O
	ATOM 6414	CB ASN H 111	15.564	6.183	83.529	1.00	11.03	C
	ATOM 6415	CG ASN H 111	15.239	6.188	82.034	1.00	16.38	C
	ATOM 6416	OD1 ASN H 111	14.630	7.129	81.510	1.00	17.18	O
	ATOM 6417	ND2 ASN H 111	15.683	5.153	81.333	1.00	17.14	N
	ATOM 6418	N ASN H 112	15.676	9.530	85.153	1.00	8.07	N
	ATOM 6419	CA ASN H 112	14.813	10.549	85.756	1.00	7.55	C
	ATOM 6420	C ASN H 112	13.951	11.218	84.688	1.00	7.89	C
	ATOM 6421	O ASN H 112	14.464	11.811	83.737	1.00	8.98	O
	ATOM 6422	CB ASN H 112	15.644	11.632	86.462	1.00	5.99	C
	ATOM 6423	CG ASN H 112	16.641	11.067	87.467	1.00	5.37	C

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FIG. 53-99	ATOM 6425 ND2 ASN H112	17.921	11.173	87.148	1.00	2.00	N
	ATOM 6426 N GLY H113	12.639	11.153	84.863	1.00	9.15	N
	ATOM 6427 CA GLY H113	11.733	11.765	83.907	1.00	9.70	C
	ATOM 6428 C GLY H113	11.526	13.268	84.031	1.00	9.37	C
	ATOM 6429 O GLY H113	11.079	13.898	83.079	1.00	10.86	O
	ATOM 6430 N PHE H114	11.822	13.851	85.189	1.00	9.22	N
	ATOM 6431 CA PHE H114	11.626	15.292	85.372	1.00	8.10	C
	ATOM 6432 C PHE H114	12.732	16.074	84.653	1.00	8.34	C
	ATOM 6433 O PHE H114	13.664	15.467	84.105	1.00	9.11	O
	ATOM 6434 CB PHE H114	11.533	15.660	86.872	1.00	6.12	C
	ATOM 6435 CG PHE H114	12.770	15.328	87.662	1.00	4.82	C
	ATOM 6436 CD1 PHE H114	12.910	14.076	88.261	1.00	2.00	C
	ATOM 6437 CD2 PHE H114	13.805	16.256	87.789	1.00	2.00	C
	ATOM 6438 CE1 PHE H114	14.060	13.743	88.974	1.00	2.00	C
	ATOM 6439 CE2 PHE H114	14.959	15.932	88.499	1.00	4.28	C
	ATOM 6440 CZ PHE H114	15.085	14.661	89.098	1.00	2.99	C
	ATOM 6441 N LEU H115	12.643	17.408	84.677	1.00	6.85	N
	ATOM 6442 CA LEU H115	13.607	18.272	84.000	1.00	5.32	C
	ATOM 6443 C LEU H115	14.176	19.366	84.918	1.00	6.67	C
	ATOM 6444 O LEU H115	13.459	20.266	85.360	1.00	7.52	O
	ATOM 6445 CB LEU H115	12.930	18.899	82.792	1.00	3.62	C
	ATOM 6446 CG LEU H115	12.123	17.922	81.946	1.00	2.00	C
	ATOM 6447 CD1 LEU H115	10.991	18.632	81.234	1.00	2.33	C
	ATOM 6448 CD2 LEU H115	13.041	17.237	80.971	1.00	4.15	C
	ATOM 6449 N LYS H116	15.490	19.318	85.124	1.00	7.90	N
	ATOM 6450 CA LYS H116	16.214	20.236	86.000	1.00	8.29	C
	ATOM 6451 C LYS H116	16.742	21.483	85.307	1.00	8.65	C
	ATOM 6452 O LYS H116	16.731	22.571	85.887	1.00	6.26	O
	ATOM 6453 CB LYS H116	17.387	19.486	86.640	1.00	8.77	C
	ATOM 6454 CG LYS H116	18.337	20.313	87.510	1.00	9.73	C
	ATOM 6455 CD LYS H116	17.703	20.766	88.803	1.00	10.23	C
	ATOM 6456 CE LYS H116	18.755	21.216	89.822	1.00	13.09	C
	ATOM 6457 NZ LYS H116	19.257	20.107	90.704	1.00	11.05	N
	ATOM 6458 N HIS H117	17.290	21.302	84.108	1.00	9.62	N
	ATOM 6459 CA HIS H117	17.847	22.414	83.349	1.00	9.20	C
	ATOM 6460 C HIS H117	17.001	22.697	82.124	1.00	8.69	C
	ATOM 6461 O HIS H117	16.453	21.787	81.524	1.00	9.06	O
	ATOM 6462 CB HIS H117	19.285	22.112	82.931	1.00	9.50	C
	ATOM 6463 CG HIS H117	20.171	21.707	84.069	1.00	13.01	C
	ATOM 6464 ND1 HIS H117	20.574	22.552	85.080	1.00	14.89	N
	ATOM 6465 CD2 HIS H117	20.713	20.499	84.367	1.00	12.49	C
	ATOM 6466 CE1 HIS H117	21.323	21.847	85.936	1.00	12.68	C
	ATOM 6467 NE2 HIS H117	21.438	20.592	85.545	1.00	13.22	N
	ATOM 6468 N TRP H118	16.882	23.968	81.768	1.00	8.39	N
	ATOM 6469 CA TRP H118	16.108	24.359	80.600	1.00	7.76	C
	ATOM 6470 C TRP H118	16.898	25.347	79.740	1.00	6.56	C
	ATOM 6471 O TRP H118	17.981	25.784	80.128	1.00	5.39	O
	ATOM 6472 CB TRP H118	14.781	24.983	81.027	1.00	7.76	C
	ATOM 6473 CG TRP H118	13.827	24.030	81.689	1.00	3.56	C
	ATOM 6474 CD1 TRP H118	13.903	23.539	82.953	1.00	4.13	C
	ATOM 6475 CD2 TRP H118	12.601	23.535	81.143	1.00	2.00	C
	ATOM 6476 NE1 TRP H118	12.794	22.782	83.240	1.00	2.00	N
	ATOM 6477 CE2 TRP H118	11.980	22.766	82.144	1.00	2.00	C
	ATOM 6478 CE3 TRP H118	11.967	23.674	79.909	1.00	2.00	C
	ATOM 6479 CZ2 TRP H118	10.753	22.141	81.946	1.00	3.79	C
	ATOM 6480 CZ3 TRP H118	10.756	23.053	79.715	1.00	2.00	C
	ATOM 6481 CH2 TRP H118	10.158	22.296	80.728	1.00	2.64	C
	ATOM 6482 N GLY H119	16.374	25.655	78.559	1.00	6.44	N
	ATOM 6483 CA GLY H119	17.035	26.585	77.664	1.00	7.62	C
	ATOM 6484 C GLY H119	16.254	27.879	77.536	1.00	8.65	C
	ATOM 6485 O GLY H119	15.098	27.949	77.953	1.00	10.48	O
	ATOM 6486 N GLN H120	16.876	28.909	76.963	1.00	10.80	N
	ATOM 6487 CA GLN H120	16.216	30.214	76.798	1.00	10.30	C
	ATOM 6488 C GLN H120	14.976	30.124	75.931	1.00	8.85	C
	ATOM 6489 O GLN H120	14.055	30.929	76.079	1.00	9.21	O
	ATOM 6490 CB GLN H120	17.158	31.247	76.194	1.00	8.92	C
	ATOM 6491 CG GLN H120	17.334	31.102	74.704	1.00	10.45	C
	ATOM 6492 CD GLN H120	18.639	30.437	74.332	1.00	12.55	C
	ATOM 6493 OE1 GLN H120	19.326	29.855	75.177	1.00	10.90	O
	ATOM 6494 NE2 GLN H120	18.000	30.522	73.054	1.00	12.02	N

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FIG. 53-100	ATOM 6496	CA GLY H 121	13.839	28.985	74.135	1.00	6.60	C
	ATOM 6497	C GLY H 121	14.180	29.405	72.729	1.00	6.68	C
	ATOM 6498	O GLY H 121	15.033	30.268	72.518	1.00	8.82	O
	ATOM 6499	N THR H 122	13.547	28.757	71.763	1.00	5.74	N
	ATOM 6500	CA THR H 122	13.766	29.059	70.369	1.00	6.29	C
	ATOM 6501	C THR H 122	12.391	29.208	69.782	1.00	8.39	C
	ATOM 6502	O THR H 122	11.602	28.262	69.818	1.00	11.50	O
	ATOM 6503	CB THR H 122	14.463	27.900	69.679	1.00	6.38	C
	ATOM 6504	OG1 THR H 122	15.664	27.599	70.382	1.00	11.11	O
	ATOM 6505	CG2 THR H 122	14.813	28.245	68.261	1.00	4.29	C
	ATOM 6506	N LEU H 123	12.048	30.411	69.336	1.00	7.48	N
	ATOM 6507	CA LEU H 123	10.735	30.592	68.740	1.00	7.17	C
	ATOM 6508	C LEU H 123	10.799	30.123	67.302	1.00	6.63	C
	ATOM 6509	O LEU H 123	11.748	30.442	66.584	1.00	6.20	O
	ATOM 6510	CB LEU H 123	10.277	32.045	68.765	1.00	6.20	C
	ATOM 6511	CG LEU H 123	8.911	32.153	68.087	1.00	5.67	C
	ATOM 6512	CD1 LEU H 123	7.887	31.381	68.902	1.00	2.00	C
	ATOM 6513	CD2 LEU H 123	8.505	33.612	67.928	1.00	8.02	C
	ATOM 6514	N VAL H 124	9.814	29.318	66.917	1.00	6.22	N
	ATOM 6515	CA VAL H 124	9.710	28.801	65.566	1.00	4.41	C
	ATOM 6516	C VAL H 124	8.327	29.187	65.103	1.00	5.26	C
	ATOM 6517	O VAL H 124	7.327	28.713	65.655	1.00	4.50	O
	ATOM 6518	CB VAL H 124	9.825	27.266	65.510	1.00	3.42	C
	ATOM 6519	CG1 VAL H 124	9.580	26.778	64.091	1.00	4.69	C
	ATOM 6520	CG2 VAL H 124	11.200	26.810	65.978	1.00	2.89	C
	ATOM 6521	N THR H 125	8.269	30.095	64.134	1.00	5.24	N
	ATOM 6522	CA THR H 125	6.997	30.547	63.591	1.00	5.65	C
	ATOM 6523	C THR H 125	6.866	29.888	62.233	1.00	5.34	C
	ATOM 6524	O THR H 125	7.829	29.869	61.453	1.00	3.74	O
	ATOM 6525	CB THR H 125	6.963	32.081	63.363	1.00	5.97	C
	ATOM 6526	OG1 THR H 125	7.710	32.750	64.386	1.00	8.20	O
	ATOM 6527	CG2 THR H 125	5.522	32.572	63.410	1.00	5.65	C
	ATOM 6528	N VAL H 126	5.692	29.327	61.967	1.00	4.89	N
	ATOM 6529	CA VAL H 126	5.441	28.672	60.700	1.00	5.00	C
	ATOM 6530	C VAL H 126	4.238	29.367	60.101	1.00	5.63	C
	ATOM 6531	O VAL H 126	3.140	29.301	60.662	1.00	4.20	O
	ATOM 6532	CB VAL H 126	5.143	27.175	60.890	1.00	5.78	C
	ATOM 6533	CG1 VAL H 126	5.045	26.490	59.529	1.00	5.45	C
	ATOM 6534	CG2 VAL H 126	6.234	26.513	61.760	1.00	4.07	C
	ATOM 6535	N THR H 127	4.450	30.067	58.987	1.00	7.29	N
	ATOM 6536	CA THR H 127	3.377	30.813	58.334	1.00	10.19	C
	ATOM 6537	C THR H 127	3.686	31.061	56.867	1.00	11.09	C
	ATOM 6538	O THR H 127	4.841	31.325	56.496	1.00	11.77	O
	ATOM 6539	CB THR H 127	3.193	32.237	58.947	1.00	11.86	C
	ATOM 6540	OG1 THR H 127	3.308	32.192	60.375	1.00	18.89	O
	ATOM 6541	CG2 THR H 127	1.830	32.821	58.576	1.00	11.36	C
	ATOM 6542	N SER H 128	2.622	31.078	56.065	1.00	10.84	N
	ATOM 6543	CA SER H 128	2.690	31.339	54.634	1.00	10.37	C
	ATOM 6544	C SER H 128	3.056	32.802	54.374	1.00	10.64	C
	ATOM 6545	O SER H 128	3.520	33.139	53.292	1.00	11.41	O
	ATOM 6546	CB SER H 128	1.333	31.054	54.017	1.00	11.13	C
	ATOM 6547	OG SER H 128	0.312	31.613	54.834	1.00	12.99	O
	ATOM 6548	N ALA H 129	2.834	33.664	55.364	1.00	11.65	N
	ATOM 6549	CA ALA H 129	3.147	35.094	55.260	1.00	13.12	C
	ATOM 6550	C ALA H 129	4.649	35.359	55.207	1.00	14.65	C
	ATOM 6551	O ALA H 129	5.431	34.589	55.759	1.00	16.91	O
	ATOM 6552	CB ALA H 129	2.540	35.841	56.420	1.00	11.97	C
	ATOM 6553	N SER H 130	5.046	36.453	54.560	1.00	15.13	N
	ATOM 6554	CA SER H 130	6.465	36.818	54.439	1.00	14.25	C
	ATOM 6555	C SER H 130	6.849	37.928	55.413	1.00	12.80	C
	ATOM 6556	O SER H 130	5.993	38.666	55.901	1.00	11.17	O
	ATOM 6557	CB SER H 130	6.782	37.271	53.011	1.00	14.65	C
	ATOM 6558	OG SER H 130	6.508	36.243	52.069	1.00	17.09	O
	ATOM 6559	N THR H 131	8.142	38.052	55.678	1.00	12.55	N
	ATOM 6560	CA THR H 131	8.659	39.067	56.598	1.00	14.01	C
	ATOM 6561	C THR H 131	8.349	40.497	56.147	1.00	14.38	C
	ATOM 6562	O THR H 131	8.318	40.796	54.944	1.00	14.04	O
	ATOM 6563	CB THR H 131	10.195	38.919	56.769	1.00	14.47	C
	ATOM 6564	OG1 THR H 131	10.510	37.582	57.185	1.00	12.21	O
	ATOM 6565	CG2 THR H 131	10.718	38.014	57.802	1.00	14.10	C

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FIG. 53-101	ATOM 6567	CA	LYS	H132	7.823	42.770	56.819	1.00	15.47	C
	ATOM 6568	C	LYS	H132	7.781	43.637	58.072	1.00	16.55	C
	ATOM 6569	O	LYS	H132	7.291	43.205	59.139	1.00	17.63	O
	ATOM 6570	CB	LYS	H132	6.513	42.915	56.037	1.00	15.09	C
	ATOM 6571	CG	LYS	H132	5.242	42.780	56.850	1.00	16.23	C
	ATOM 6572	CD	LYS	H132	4.027	43.112	55.997	1.00	16.20	C
	ATOM 6573	CE	LYS	H132	4.057	44.551	55.500	1.00	16.81	C
	ATOM 6574	NZ	LYS	H132	3.995	45.539	56.630	1.00	21.10	N
	ATOM 6575	N	GLY	H133	8.348	44.837	57.947	1.00	15.20	N
	ATOM 6576	CA	GLY	H133	8.363	45.790	59.042	1.00	12.03	C
	ATOM 6577	C	GLY	H133	6.963	46.314	59.284	1.00	9.06	C
	ATOM 6578	O	GLY	H133	6.141	46.329	58.366	1.00	9.32	O
	ATOM 6579	N	PRO	H134	6.660	46.765	60.502	1.00	7.19	N
	ATOM 6580	CA	PRO	H134	5.326	47.273	60.806	1.00	7.38	C
	ATOM 6581	C	PRO	H134	5.055	48.719	60.416	1.00	8.86	C
	ATOM 6582	O	PRO	H134	5.958	49.476	60.028	1.00	7.17	O
	ATOM 6583	CB	PRO	H134	5.250	47.103	62.312	1.00	6.38	C
	ATOM 6584	CG	PRO	H134	6.640	47.479	62.730	1.00	6.33	C
	ATOM 6585	CD	PRO	H134	7.510	46.766	61.706	1.00	7.21	C
	ATOM 6586	N	SER	H135	3.778	49.075	60.529	1.00	10.15	N
	ATOM 6587	CA	SER	H135	3.281	50.404	60.252	1.00	9.30	C
	ATOM 6588	C	SER	H135	3.074	51.015	61.616	1.00	9.91	C
	ATOM 6589	O	SER	H135	2.216	50.569	62.373	1.00	10.72	O
	ATOM 6590	CB	SER	H135	1.927	50.333	59.545	1.00	9.06	C
	ATOM 6591	OG	SER	H135	2.054	49.874	58.212	1.00	12.48	O
	ATOM 6592	N	VAL	H136	3.903	51.983	61.964	1.00	10.98	N
	ATOM 6593	CA	VAL	H136	3.765	52.641	63.244	1.00	11.00	C
	ATOM 6594	C	VAL	H136	2.875	53.876	63.099	1.00	10.33	C
	ATOM 6595	O	VAL	H136	3.197	54.806	62.363	1.00	8.56	O
	ATOM 6596	CB	VAL	H136	5.136	53.037	63.814	1.00	13.40	C
	ATOM 6597	CG1	VAL	H136	4.974	53.698	65.193	1.00	13.53	C
	ATOM 6598	CG2	VAL	H136	6.029	51.803	63.905	1.00	14.01	C
	ATOM 6599	N	PHE	H137	1.733	53.843	63.776	1.00	11.17	N
	ATOM 6600	CA	PHE	H137	0.773	54.942	63.790	1.00	11.79	C
	ATOM 6601	C	PHE	H137	0.656	55.374	65.250	1.00	13.75	C
	ATOM 6602	O	PHE	H137	0.747	54.547	66.148	1.00	12.53	O
	ATOM 6603	CB	PHE	H137	-0.597	54.469	63.293	1.00	11.07	C
	ATOM 6604	CG	PHE	H137	-0.577	53.926	61.906	1.00	10.97	C
	ATOM 6605	CD1	PHE	H137	-0.157	54.723	60.840	1.00	12.08	C
	ATOM 6606	CD2	PHE	H137	-0.954	52.613	61.659	1.00	10.56	C
	ATOM 6607	CE1	PHE	H137	-0.112	54.215	59.545	1.00	10.06	C
	ATOM 6608	CE2	PHE	H137	-0.914	52.097	60.375	1.00	10.49	C
	ATOM 6609	CZ	PHE	H137	-0.493	52.898	59.316	1.00	10.89	C
	ATOM 6610	N	PRO	H138	0.458	56.676	65.507	1.00	15.89	N
	ATOM 6611	CA	PRO	H138	0.336	57.195	66.870	1.00	18.02	C
	ATOM 6612	C	PRO	H138	-1.116	57.271	67.323	1.00	20.61	C
	ATOM 6613	O	PRO	H138	-2.028	57.423	66.502	1.00	22.40	O
	ATOM 6614	CB	PRO	H138	0.915	58.588	66.728	1.00	17.19	C
	ATOM 6615	CG	PRO	H138	0.306	59.018	65.429	1.00	17.20	C
	ATOM 6616	CD	PRO	H138	0.434	57.780	64.532	1.00	16.18	C
	ATOM 6617	N	LEU	H139	-1.320	57.182	68.636	1.00	22.53	N
	ATOM 6618	CA	LEU	H139	-2.647	57.256	69.243	1.00	24.41	C
	ATOM 6619	C	LEU	H139	-2.765	58.622	69.912	1.00	26.20	C
	ATOM 6620	O	LEU	H139	-2.600	58.752	71.120	1.00	25.66	O
	ATOM 6621	CB	LEU	H139	-2.812	56.130	70.266	1.00	22.44	C
	ATOM 6622	CG	LEU	H139	-3.492	54.850	69.786	1.00	21.57	C
	ATOM 6623	CD1	LEU	H139	-3.350	54.682	68.286	1.00	21.35	C
	ATOM 6624	CD2	LEU	H139	-2.921	53.658	70.536	1.00	20.98	C
	ATOM 6625	N	ALA	H140	-2.990	59.640	69.089	1.00	30.01	N
	ATOM 6626	CA	ALA	H140	-3.104	61.027	69.534	1.00	31.42	C
	ATOM 6627	C	ALA	H140	-3.967	61.181	70.768	1.00	32.96	C
	ATOM 6628	O	ALA	H140	-5.041	60.575	70.865	1.00	32.60	O
	ATOM 6629	CB	ALA	H140	-3.643	61.908	68.399	1.00	31.26	C
	ATOM 6630	N	PRO	H141	-3.502	61.996	71.736	1.00	34.92	N
	ATOM 6631	CA	PRO	H141	-4.200	62.264	72.997	1.00	36.69	C
	ATOM 6632	C	PRO	H141	-5.699	62.466	72.814	1.00	38.82	C
	ATOM 6633	O	PRO	H141	-6.135	63.500	72.312	1.00	38.07	O
	ATOM 6634	CB	PRO	H141	-3.512	63.532	73.492	1.00	35.13	C
	ATOM 6635	CG	PRO	H141	-2.094	63.290	73.100	1.00	33.37	C
	ATOM 6636	CD	PRO	H141	-2.225	62.727	71.685	1.00	32.66	C

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FIG. 53-102

ATOM 6638	CA	SER H 142	-7.924	61.421	73.169	1.00	44.81	C
ATOM 6639	C	SER H 142	-8.580	62.786	73.342	1.00	46.31	C
ATOM 6640	O	SER H 142	-9.637	63.057	72.768	1.00	47.19	O
ATOM 6641	CB	SER H 142	-8.463	60.442	74.214	1.00	45.28	C
ATOM 6642	OG	SER H 142	-7.701	60.515	75.412	1.00	45.59	O
ATOM 6643	N	SER H 143	-7.943	63.617	74.158	1.00	47.43	N
ATOM 6644	CA	SER H 143	-8.357	64.979	74.460	1.00	48.43	C
ATOM 6645	C	SER H 143	-7.504	65.399	75.643	1.00	48.58	C
ATOM 6646	O	SER H 143	-7.116	64.559	76.459	1.00	48.13	O
ATOM 6647	CB	SER H 143	-9.846	65.061	74.821	1.00	49.31	C
ATOM 6648	OG	SER H 143	-10.651	65.255	73.666	1.00	50.90	O
ATOM 6649	N	LYSH 144	-7.167	66.683	75.709	1.00	49.12	N
ATOM 6650	CA	LYSH 144	-6.349	67.202	76.800	1.00	49.89	C
ATOM 6651	C	LYSH 144	-6.844	66.662	78.140	1.00	51.31	C
ATOM 6652	O	LYSH 144	-6.090	66.025	78.869	1.00	51.30	O
ATOM 6653	CB	LYSH 144	-6.360	68.734	76.790	1.00	49.53	C
ATOM 6654	CG	LYSH 144	-5.683	69.354	75.575	1.00	48.06	C
ATOM 6655	CD	LYSH 144	-4.186	69.080	75.567	1.00	46.41	C
ATOM 6656	CE	LYSH 144	-3.546	69.638	74.306	1.00	45.68	C
ATOM 6657	NZ	LYSH 144	-2.062	69.598	74.338	1.00	43.77	N
ATOM 6658	N	SER H 145	-8.114	66.901	78.452	1.00	52.64	N
ATOM 6659	CA	SER H 145	-8.684	66.399	79.694	1.00	53.40	C
ATOM 6660	C	SER H 145	-9.201	64.985	79.410	1.00	52.91	C
ATOM 6661	O	SER H 145	-9.725	64.713	78.321	1.00	52.97	O
ATOM 6662	CB	SER H 145	-9.821	67.306	80.178	1.00	53.39	C
ATOM 6663	OG	SER H 145	-9.400	68.652	80.327	1.00	54.54	O
ATOM 6664	N	THR H 146	-9.018	64.086	80.371	1.00	51.26	N
ATOM 6665	CA	THR H 146	-9.450	62.701	80.234	1.00	49.59	C
ATOM 6666	C	THR H 146	-9.988	62.200	81.572	1.00	49.59	C
ATOM 6667	O	THR H 146	-10.211	62.993	82.493	1.00	49.78	O
ATOM 6668	CB	THR H 146	-8.270	61.814	79.808	1.00	48.67	C
ATOM 6669	OG1	THR H 146	-7.096	62.216	80.523	1.00	47.79	O
ATOM 6670	CG2	THR H 146	-8.021	61.923	78.309	1.00	48.73	C
ATOM 6671	N	SER H 147	-10.226	60.893	81.675	1.00	48.75	N
ATOM 6672	CA	SER H 147	-10.729	60.307	82.915	1.00	48.48	C
ATOM 6673	C	SER H 147	-9.705	60.452	84.038	1.00	48.25	C
ATOM 6674	O	SER H 147	-8.741	59.683	84.120	1.00	48.10	O
ATOM 6675	CB	SER H 147	-11.084	58.830	82.714	1.00	48.05	C
ATOM 6676	OG	SER H 147	-12.328	58.685	82.040	1.00	48.59	O
ATOM 6677	N	GLY H 148	-9.905	61.464	84.878	1.00	47.37	N
ATOM 6678	CA	GLY H 148	-9.002	61.708	85.989	1.00	45.76	C
ATOM 6679	C	GLY H 148	-8.209	62.980	85.779	1.00	44.78	C
ATOM 6680	O	GLY H 148	-8.181	63.845	86.644	1.00	44.91	O
ATOM 6681	N	GLY H 149	-7.554	63.086	84.629	1.00	43.88	N
ATOM 6682	CA	GLY H 149	-6.772	64.273	84.333	1.00	42.23	C
ATOM 6683	C	GLY H 149	-5.403	63.928	83.793	1.00	40.65	C
ATOM 6684	O	GLY H 149	-4.541	64.800	83.623	1.00	40.43	O
ATOM 6685	N	THR H 150	-5.210	62.642	83.537	1.00	39.02	N
ATOM 6686	CA	THR H 150	-3.963	62.119	83.016	1.00	36.37	C
ATOM 6687	C	THR H 150	-4.241	61.693	81.581	1.00	34.47	C
ATOM 6688	O	THR H 150	-5.009	60.757	81.337	1.00	34.73	O
ATOM 6689	CB	THR H 150	-3.477	60.881	83.842	1.00	36.14	C
ATOM 6690	OG1	THR H 150	-3.512	61.180	85.248	1.00	32.44	O
ATOM 6691	CG2	THR H 150	-2.051	60.496	83.455	1.00	35.60	C
ATOM 6692	N	ALA H 151	-3.677	62.424	80.630	1.00	32.10	N
ATOM 6693	CA	ALA H 151	-3.851	62.098	79.227	1.00	30.67	C
ATOM 6694	C	ALA H 151	-3.236	60.725	78.973	1.00	30.16	C
ATOM 6695	O	ALA H 151	-2.532	60.176	79.827	1.00	29.46	O
ATOM 6696	CB	ALA H 151	-3.168	63.150	78.352	1.00	29.03	C
ATOM 6697	N	ALA H 152	-3.531	60.163	77.810	1.00	29.66	N
ATOM 6698	CA	ALA H 152	-2.993	58.870	77.422	1.00	28.48	C
ATOM 6699	C	ALA H 152	-2.818	58.876	75.914	1.00	27.26	C
ATOM 6700	O	ALA H 152	-3.712	59.305	75.181	1.00	27.16	O
ATOM 6701	CB	ALA H 152	-3.935	57.748	77.844	1.00	29.31	C
ATOM 6702	N	LEU H 153	-1.636	58.480	75.466	1.00	26.25	N
ATOM 6703	CA	LEU H 153	-1.332	58.415	74.043	1.00	25.79	C
ATOM 6704	C	LEU H 153	-0.510	57.154	73.767	1.00	24.66	C
ATOM 6705	O	LEU H 153	-0.178	56.417	74.696	1.00	24.12	O
ATOM 6706	CB	LEU H 153	-0.605	59.693	73.567	1.00	26.39	C
ATOM 6707	CG	LEU H 153	-0.658	60.312	74.186	1.00	25.06	C

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FIG. 53-103

ATOM 6709	CD2 LEU H 153	1.847	59.368	74.110	1.00	28.30	C
ATOM 6710	N GLY H 154	-0.213	56.880	72.502	1.00	23.70	N
ATOM 6711	CA GLY H 154	0.568	55.697	72.199	1.00	22.99	C
ATOM 6712	C GLY H 154	0.875	55.459	70.737	1.00	22.92	C
ATOM 6713	O GLY H 154	0.891	56.396	69.927	1.00	21.74	O
ATOM 6714	N CYSH 155	1.088	54.190	70.398	1.00	22.73	N
ATOM 6715	CA CYSH 155	1.406	53.791	69.035	1.00	21.51	C
ATOM 6716	C CYSH 155	0.773	52.453	68.655	1.00	20.37	C
ATOM 6717	O CYSH 155	0.755	51.514	69.458	1.00	21.44	O
ATOM 6718	CB CYSH 155	2.928	53.684	68.853	1.00	22.18	C
ATOM 6719	SG CYSH 155	3.784	55.277	68.636	1.00	25.02	S
ATOM 6720	N LEU H 156	0.194	52.407	67.459	1.00	17.40	N
ATOM 6721	CA LEU H 156	-0.396	51.203	66.903	1.00	14.77	C
ATOM 6722	C LEU H 156	0.707	50.685	65.992	1.00	13.15	C
ATOM 6723	O LEU H 156	1.110	51.366	65.050	1.00	11.25	O
ATOM 6724	CB LEU H 156	-1.646	51.530	66.065	1.00	14.58	C
ATOM 6725	CG LEU H 156	-2.451	50.371	65.437	1.00	13.68	C
ATOM 6726	CD1 LEU H 156	-3.148	49.517	66.505	1.00	12.41	C
ATOM 6727	CD2 LEU H 156	-3.485	50.923	64.475	1.00	10.42	C
ATOM 6728	N VAL H 157	1.267	49.533	66.343	1.00	13.00	N
ATOM 6729	CA VAL H 157	2.329	48.913	65.561	1.00	10.97	C
ATOM 6730	C VAL H 157	1.674	47.722	64.892	1.00	10.83	C
ATOM 6731	O VAL H 157	1.675	46.626	65.449	1.00	13.03	O
ATOM 6732	CB VAL H 157	3.463	48.425	66.469	1.00	10.06	C
ATOM 6733	CG1 VAL H 157	4.626	47.971	65.649	1.00	9.37	C
ATOM 6734	CG2 VAL H 157	3.887	49.530	67.421	1.00	12.85	C
ATOM 6735	N LYSH 158	1.100	47.943	63.710	1.00	9.96	N
ATOM 6736	CA LYSH 158	0.398	46.889	62.993	1.00	8.89	C
ATOM 6737	C LYSH 158	0.992	46.427	61.655	1.00	9.25	C
ATOM 6738	O LYSH 158	1.905	47.043	61.107	1.00	9.17	O
ATOM 6739	CB LYSH 158	-1.081	47.277	62.828	1.00	7.35	C
ATOM 6740	CG LYSH 158	-1.459	47.925	61.516	1.00	4.06	C
ATOM 6741	CD LYSH 158	-2.926	48.374	61.537	1.00	2.31	C
ATOM 6742	CE LYSH 158	-3.910	47.219	61.613	1.00	2.00	C
ATOM 6743	NZ LYSH 158	-4.065	46.520	60.303	1.00	4.12	N
ATOM 6744	N ASP H 159	0.487	45.288	61.186	1.00	10.34	N
ATOM 6745	CA ASP H 159	0.883	44.650	59.938	1.00	9.94	C
ATOM 6746	C ASP H 159	2.340	44.239	59.779	1.00	10.44	C
ATOM 6747	O ASP H 159	2.940	44.406	58.708	1.00	10.80	O
ATOM 6748	CB ASP H 159	0.383	45.448	58.733	1.00	9.84	C
ATOM 6749	CG ASP H 159	-1.138	45.491	58.658	1.00	12.75	C
ATOM 6750	OD1 ASP H 159	-1.806	44.831	59.489	1.00	11.14	O
ATOM 6751	OD2 ASP H 159	-1.687	46.194	57.782	1.00	14.15	O
ATOM 6752	N TYR H 160	2.906	43.680	60.845	1.00	11.17	N
ATOM 6753	CA TYR H 160	4.285	43.184	60.809	1.00	12.41	C
ATOM 6754	C TYR H 160	4.167	41.673	60.919	1.00	11.93	C
ATOM 6755	O TYR H 160	3.183	41.164	61.464	1.00	10.90	O
ATOM 6756	CB TYR H 160	5.160	43.768	61.933	1.00	12.71	C
ATOM 6757	CG TYR H 160	4.765	43.387	63.337	1.00	13.00	C
ATOM 6758	CD1 TYR H 160	3.718	44.035	63.984	1.00	13.98	C
ATOM 6759	CD2 TYR H 160	5.451	42.385	64.029	1.00	12.39	C
ATOM 6760	CE1 TYR H 160	3.362	43.698	65.291	1.00	13.65	C
ATOM 6761	CE2 TYR H 160	5.106	42.047	65.326	1.00	11.41	C
ATOM 6762	CZ TYR H 160	4.062	42.705	65.956	1.00	11.70	C
ATOM 6763	OH TYR H 160	3.719	42.379	67.250	1.00	12.51	O
ATOM 6764	N PHE H 161	5.137	40.948	60.374	1.00	13.91	N
ATOM 6765	CA PHE H 161	5.042	39.501	60.418	1.00	15.66	C
ATOM 6766	C PHE H 161	5.775	38.788	61.543	1.00	17.16	C
ATOM 6767	O PHE H 161	5.145	38.450	62.549	1.00	19.68	O
ATOM 6768	CB PHE H 161	5.302	38.854	59.044	1.00	14.33	C
ATOM 6769	CG PHE H 161	5.267	37.354	59.073	1.00	12.76	C
ATOM 6770	CD1 PHE H 161	4.191	36.688	59.644	1.00	12.11	C
ATOM 6771	CD2 PHE H 161	6.352	36.607	58.619	1.00	12.73	C
ATOM 6772	CE1 PHE H 161	4.201	35.301	59.764	1.00	11.53	C
ATOM 6773	CE2 PHE H 161	6.369	35.220	58.735	1.00	10.89	C
ATOM 6774	CZ PHE H 161	5.297	34.567	59.313	1.00	10.41	C
ATOM 6775	N PRO H 162	7.096	38.532	61.412	1.00	16.48	N
ATOM 6776	CA PRO H 162	7.687	37.832	62.559	1.00	15.52	C
ATOM 6777	C PRO H 162	7.440	38.626	63.839	1.00	16.26	C
ATOM 6778	O PRO H 162	7.717	38.822	62.896	1.00	15.76	O



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FIG. 53-104	ATOM 6780 CG PRO H 162	9.121	37.678	60.688	1.00	15.53	C
	ATOM 6781 CD PRO H 162	8.115	38.768	60.375	1.00	15.70	C
	ATOM 6782 N GLNH 163	6.838	37.953	64.821	1.00	17.27	N
	ATOM 6783 CA GLNH 163	6.465	38.532	66.112	1.00	18.22	C
	ATOM 6784 C GLNH 163	7.433	39.454	66.869	1.00	18.88	C
	ATOM 6785 O GLNH 163	7.040	40.541	67.326	1.00	19.04	O
	ATOM 6786 CB GLNH 163	5.993	37.428	67.058	1.00	18.98	C
	ATOM 6787 CG GLNH 163	4.617	37.668	67.637	1.00	18.94	C
	ATOM 6788 CD GLNH 163	4.561	38.878	68.535	1.00	19.62	C
	ATOM 6789 OE1 GLNH 163	4.408	38.753	69.752	1.00	21.57	O
	ATOM 6790 NE2 GLNH 163	4.667	40.062	67.947	1.00	17.24	N
	ATOM 6791 N PRO H 164	8.697	39.036	67.022	1.00	17.42	N
	ATOM 6792 CA PRO H 164	9.683	39.851	67.741	1.00	16.50	C
	ATOM 6793 C PRO H 164	9.767	41.348	67.396	1.00	16.72	C
	ATOM 6794 O PRO H 164	10.544	41.766	66.526	1.00	15.30	O
	ATOM 6795 CB PRO H 164	10.992	39.117	67.465	1.00	17.30	C
	ATOM 6796 CG PRO H 164	10.703	38.336	66.175	1.00	17.74	C
	ATOM 6797 CD PRO H 164	9.327	37.847	66.419	1.00	15.64	C
	ATOM 6798 N VAL H 165	8.979	42.147	68.120	1.00	17.00	N
	ATOM 6799 CA VAL H 165	8.946	43.604	67.968	1.00	14.97	C
	ATOM 6800 C VAL H 165	9.136	44.216	69.370	1.00	14.98	C
	ATOM 6801 O VAL H 165	8.626	43.680	70.360	1.00	15.43	O
	ATOM 6802 CB VAL H 165	7.600	44.100	67.334	1.00	12.34	C
	ATOM 6803 CG1 VAL H 165	6.629	44.578	68.403	1.00	10.73	C
	ATOM 6804 CG2 VAL H 165	7.861	45.207	66.331	1.00	10.36	C
	ATOM 6805 N THR H 166	9.928	45.283	69.458	1.00	14.94	N
	ATOM 6806 CA THR H 166	10.173	45.969	70.732	1.00	14.09	C
	ATOM 6807 C THR H 166	9.767	47.421	70.588	1.00	13.15	C
	ATOM 6808 O THR H 166	10.005	48.033	69.547	1.00	13.03	O
	ATOM 6809 CB THR H 166	11.651	45.926	71.164	1.00	14.47	C
	ATOM 6810 OG1 THR H 166	12.466	46.558	70.169	1.00	15.67	O
	ATOM 6811 CG2 THR H 166	12.107	44.490	71.373	1.00	13.84	C
	ATOM 6812 N VAL H 167	9.151	47.967	71.631	1.00	12.92	N
	ATOM 6813 CA VAL H 167	8.701	49.352	71.608	1.00	12.11	C
	ATOM 6814 C VAL H 167	9.166	50.088	72.854	1.00	10.91	C
	ATOM 6815 O VAL H 167	9.146	49.536	73.948	1.00	11.06	O
	ATOM 6816 CB VAL H 167	7.159	49.444	71.498	1.00	13.51	C
	ATOM 6817 CG1 VAL H 167	6.716	50.908	71.454	1.00	13.75	C
	ATOM 6818 CG2 VAL H 167	6.669	48.691	70.257	1.00	11.11	C
	ATOM 6819 N SER H 168	9.617	51.323	72.673	1.00	12.04	N
	ATOM 6820 CA SER H 168	10.087	52.156	73.779	1.00	12.70	C
	ATOM 6821 C SER H 168	9.495	53.551	73.632	1.00	11.89	C
	ATOM 6822 O SER H 168	8.862	53.873	72.622	1.00	10.00	O
	ATOM 6823 CB SER H 168	11.624	52.277	73.764	1.00	13.07	C
	ATOM 6824 OG SER H 168	12.261	51.022	73.603	1.00	16.68	O
	ATOM 6825 N TRP H 169	9.771	54.388	74.625	1.00	13.49	N
	ATOM 6826 CA TRP H 169	9.307	55.769	74.659	1.00	14.33	C
	ATOM 6827 C TRP H 169	10.484	56.641	75.061	1.00	13.65	C
	ATOM 6828 O TRP H 169	11.248	56.284	75.972	1.00	13.91	O
	ATOM 6829 CB TRP H 169	8.173	55.929	75.669	1.00	16.34	C
	ATOM 6830 CG TRP H 169	6.913	55.288	75.213	1.00	19.47	C
	ATOM 6831 CD1 TRP H 169	6.441	54.060	75.562	1.00	19.30	C
	ATOM 6832 CD2 TRP H 169	5.985	55.820	74.259	1.00	21.40	C
	ATOM 6833 NE1 TRP H 169	5.284	53.784	74.877	1.00	22.35	N
	ATOM 6834 CE2 TRP H 169	4.979	54.850	74.070	1.00	22.25	C
	ATOM 6835 CE3 TRP H 169	5.910	57.022	73.539	1.00	23.11	C
	ATOM 6836 CZ2 TRP H 169	3.907	55.045	73.191	1.00	22.21	C
	ATOM 6837 CZ3 TRP H 169	4.846	57.214	72.667	1.00	22.11	C
	ATOM 6838 CH2 TRP H 169	3.861	56.229	72.501	1.00	21.83	C
	ATOM 6839 N ASN H 170	10.630	57.773	74.373	1.00	11.73	N
	ATOM 6840 CA ASN H 170	11.706	58.722	74.628	1.00	10.55	C
	ATOM 6841 C ASN H 170	13.056	58.024	74.701	1.00	10.89	C
	ATOM 6842 O ASN H 170	13.839	58.260	75.630	1.00	9.68	O
	ATOM 6843 CB ASN H 170	11.472	59.481	75.932	1.00	11.66	C
	ATOM 6844 CG ASN H 170	10.272	60.394	75.885	1.00	12.60	C
	ATOM 6845 OD1 ASN H 170	9.860	60.911	76.914	1.00	14.09	O
	ATOM 6846 ND2 ASN H 170	9.725	60.626	74.706	1.00	13.33	N
	ATOM 6847 N SER H 171	13.294	57.113	73.763	1.00	11.69	N
	ATOM 6848 CA SER H 171	14.547	56.376	73.704	1.00	12.66	C
	ATOM 6849 C SER H 171	14.077	55.806	75.070	1.00	11.52	C

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FIG. 53-105	ATOM 6851	CB SER H 171	15.617	57.293	73.128	1.00	13.68	C
	ATOM 6852	OG SER H 171	15.110	57.967	71.982	1.00	14.88	O
	ATOM 6853	N GLY H 172	13.999	55.278	75.811	1.00	11.14	N
	ATOM 6854	CA GLY H 172	14.253	54.675	77.112	1.00	9.53	C
	ATOM 6855	C GLY H 172	14.197	55.608	78.307	1.00	9.53	C
	ATOM 6856	O GLY H 172	14.357	55.167	79.452	1.00	8.14	O
	ATOM 6857	N ALA H 173	13.970	56.892	78.049	1.00	9.47	N
	ATOM 6858	CA ALA H 173	13.912	57.909	79.109	1.00	10.56	C
	ATOM 6859	C ALA H 173	12.587	57.852	79.857	1.00	10.20	C
	ATOM 6860	O ALA H 173	12.496	58.160	81.055	1.00	8.98	O
	ATOM 6861	CB ALA H 173	14.121	59.297	78.512	1.00	9.38	C
	ATOM 6862	N LEU H 174	11.551	57.500	79.110	1.00	10.48	N
	ATOM 6863	CA LEU H 174	10.214	57.369	79.642	1.00	10.25	C
	ATOM 6864	C LEU H 174	9.955	55.868	79.744	1.00	11.08	C
	ATOM 6865	O LEU H 174	10.124	55.132	78.768	1.00	11.25	O
	ATOM 6866	CB LEU H 174	9.216	58.042	78.699	1.00	6.90	C
	ATOM 6867	CG LEU H 174	7.736	57.832	78.977	1.00	5.18	C
	ATOM 6868	CD1 LEU H 174	7.406	58.185	80.411	1.00	6.39	C
	ATOM 6869	CD2 LEU H 174	6.917	58.650	78.007	1.00	4.39	C
	ATOM 6870	N THR H 175	9.630	55.416	80.950	1.00	13.76	N
	ATOM 6871	CA THR H 175	9.348	54.005	81.208	1.00	15.62	C
	ATOM 6872	C THR H 175	8.210	53.801	82.219	1.00	17.32	C
	ATOM 6873	O THR H 175	7.619	52.718	82.289	1.00	19.37	O
	ATOM 6874	CB THR H 175	10.615	53.264	81.703	1.00	13.60	C
	ATOM 6875	OG1 THR H 175	11.353	54.117	82.587	1.00	13.52	O
	ATOM 6876	CG2 THR H 175	11.502	52.870	80.532	1.00	9.95	C
	ATOM 6877	N SER H 176	7.888	54.831	82.994	1.00	17.59	N
	ATOM 6878	CA SER H 176	6.811	54.700	83.973	1.00	17.83	C
	ATOM 6879	C SER H 176	5.425	54.960	83.361	1.00	16.06	C
	ATOM 6880	O SER H 176	5.265	55.846	82.528	1.00	13.90	O
	ATOM 6881	CB SER H 176	7.058	55.604	85.190	1.00	18.75	C
	ATOM 6882	OG SER H 176	7.703	56.822	84.833	1.00	23.79	O
	ATOM 6883	N GLY H 177	4.451	54.129	83.733	1.00	15.54	N
	ATOM 6884	CA GLY H 177	3.096	54.271	83.225	1.00	15.16	C
	ATOM 6885	C GLY H 177	2.816	53.621	81.878	1.00	15.96	C
	ATOM 6886	O GLY H 177	1.648	53.469	81.494	1.00	14.91	O
	ATOM 6887	N VAL H 178	3.872	53.198	81.177	1.00	16.41	N
	ATOM 6888	CA VAL H 178	3.737	52.579	79.854	1.00	16.11	C
	ATOM 6889	C VAL H 178	3.096	51.190	79.873	1.00	15.06	C
	ATOM 6890	O VAL H 178	3.199	50.452	80.853	1.00	16.45	O
	ATOM 6891	CB VAL H 178	5.103	52.495	79.106	1.00	16.24	C
	ATOM 6892	CG1 VAL H 178	5.816	53.841	79.137	1.00	14.61	C
	ATOM 6893	CG2 VAL H 178	5.979	51.406	79.707	1.00	17.09	C
	ATOM 6894	N HIS H 179	2.451	50.842	78.769	1.00	13.81	N
	ATOM 6895	CA HIS H 179	1.770	49.563	78.612	1.00	12.20	C
	ATOM 6896	C HIS H 179	1.917	49.074	77.179	1.00	11.92	C
	ATOM 6897	O HIS H 179	1.301	49.630	76.279	1.00	10.81	O
	ATOM 6898	CB HIS H 179	0.268	49.723	78.865	1.00	10.78	C
	ATOM 6899	CG HIS H 179	-0.089	50.040	80.288	1.00	8.98	C
	ATOM 6900	ND1 HIS H 179	0.744	49.786	81.344	1.00	8.13	N
	ATOM 6901	CD2 HIS H 179	-1.230	50.550	80.810	1.00	7.69	C
	ATOM 6902	CE1 HIS H 179	0.135	50.122	82.475	1.00	7.19	C
	ATOM 6903	NE2 HIS H 179	-1.057	50.586	82.174	1.00	6.91	N
	ATOM 6904	N THR H 180	2.722	48.044	76.955	1.00	12.23	N
	ATOM 6905	CA THR H 180	2.866	47.510	75.609	1.00	13.23	C
	ATOM 6906	C THR H 180	2.130	46.173	75.592	1.00	12.61	C
	ATOM 6907	O THR H 180	2.649	45.154	76.040	1.00	13.86	O
	ATOM 6908	CB THR H 180	4.343	47.363	75.216	1.00	13.85	C
	ATOM 6909	OG1 THR H 180	4.978	48.652	75.308	1.00	14.97	O
	ATOM 6910	CG2 THR H 180	4.465	46.841	73.784	1.00	8.77	C
	ATOM 6911	N PHE H 181	0.887	46.206	75.127	1.00	11.37	N
	ATOM 6912	CA PHE H 181	0.039	45.025	75.100	1.00	10.00	C
	ATOM 6913	C PHE H 181	0.611	43.950	74.220	1.00	10.71	C
	ATOM 6914	O PHE H 181	1.166	44.243	73.168	1.00	11.45	O
	ATOM 6915	CB PHE H 181	-1.374	45.398	74.630	1.00	8.58	C
	ATOM 6916	CG PHE H 181	-2.042	46.412	75.503	1.00	6.96	C
	ATOM 6917	CD1 PHE H 181	-2.736	46.017	76.643	1.00	5.39	C
	ATOM 6918	CD2 PHE H 181	-1.904	47.767	75.243	1.00	5.58	C
	ATOM 6919	CE1 PHE H 181	-3.273	46.959	77.514	1.00	2.00	C
	ATOM 6920	CE2 PHE H 181	2.441	48.708	76.112	1.00	4.38	C

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FIG. 53-106	ATOM 6922 N PRO H 182	0.505	42.681	74.653	1.00	11.10	N
	ATOM 6923 CA PRO H 182	1.014	41.533	73.896	1.00	10.01	C
	ATOM 6924 C PRO H 182	0.447	41.543	72.495	1.00	8.35	C
	ATOM 6925 O PRO H 182	-0.682	41.975	72.282	1.00	8.98	O
	ATOM 6926 CB PRO H 182	0.472	40.341	74.688	1.00	10.33	C
	ATOM 6927 CG PRO H 182	0.481	40.839	76.085	1.00	8.56	C
	ATOM 6928 CD PRO H 182	-0.093	42.240	75.926	1.00	10.78	C
	ATOM 6929 N ALA H 183	1.225	41.056	71.543	1.00	7.01	N
	ATOM 6930 CA ALA H 183	0.789	41.014	70.153	1.00	5.50	C
	ATOM 6931 C ALA H 183	-0.441	40.154	69.880	1.00	4.29	C
	ATOM 6932 O ALA H 183	-0.716	39.167	70.571	1.00	5.06	O
	ATOM 6933 CB ALA H 183	1.924	40.560	69.276	1.00	4.84	C
	ATOM 6934 N VAL H 184	-1.168	40.539	68.847	1.00	3.67	N
	ATOM 6935 CA VAL H 184	-2.355	39.827	68.422	1.00	3.96	C
	ATOM 6936 C VAL H 184	-2.137	39.463	66.960	1.00	5.83	C
	ATOM 6937 O VAL H 184	-1.449	40.187	66.234	1.00	8.89	O
	ATOM 6938 CB VAL H 184	-3.580	40.729	68.560	1.00	3.97	C
	ATOM 6939 CG1 VAL H 184	-4.584	40.470	67.447	1.00	6.95	C
	ATOM 6940 CG2 VAL H 184	-4.220	40.506	69.907	1.00	6.37	C
	ATOM 6941 N LEU H 185	-2.656	38.316	66.536	1.00	6.33	N
	ATOM 6942 CA LEU H 185	-2.518	37.905	65.141	1.00	4.96	C
	ATOM 6943 C LEU H 185	-3.812	38.263	64.423	1.00	5.98	C
	ATOM 6944 O LEU H 185	-4.911	37.958	64.908	1.00	4.69	O
	ATOM 6945 CB LEU H 185	-2.276	36.401	65.027	1.00	3.01	C
	ATOM 6946 CG LEU H 185	-1.861	35.914	63.639	1.00	2.00	C
	ATOM 6947 CD1 LEU H 185	-0.558	36.576	63.252	1.00	2.00	C
	ATOM 6948 CD2 LEU H 185	-1.705	34.409	63.639	1.00	2.00	C
	ATOM 6949 N GLN H 186	-3.685	38.984	63.317	1.00	6.25	N
	ATOM 6950 CA GLN H 186	-4.846	39.362	62.536	1.00	7.15	C
	ATOM 6951 C GLN H 186	-5.151	38.230	61.558	1.00	8.80	C
	ATOM 6952 O GLN H 186	-4.271	37.427	61.232	1.00	9.09	O
	ATOM 6953 CB GLN H 186	-4.576	40.660	61.782	1.00	4.80	C
	ATOM 6954 CG GLN H 186	-4.362	41.856	62.690	1.00	4.42	C
	ATOM 6955 CD GLN H 186	-3.792	43.050	61.959	1.00	2.12	C
	ATOM 6956 OE1 GLN H 186	-4.382	44.142	61.954	1.00	2.81	O
	ATOM 6957 NE2 GLN H 186	-2.618	42.868	61.376	1.00	2.00	N
	ATOM 6958 N SER H 187	-6.388	38.198	61.064	1.00	9.24	N
	ATOM 6959 CA SER H 187	-6.829	37.197	60.110	1.00	8.26	C
	ATOM 6960 C SER H 187	-5.997	37.221	58.828	1.00	7.98	C
	ATOM 6961 O SER H 187	-6.087	36.311	58.006	1.00	8.54	O
	ATOM 6962 CB SER H 187	-8.304	37.416	59.794	1.00	10.14	C
	ATOM 6963 OG SER H 187	-9.040	37.613	60.998	1.00	15.53	O
	ATOM 6964 N SER H 188	-5.205	38.272	58.648	1.00	7.78	N
	ATOM 6965 CA SER H 188	-4.338	38.390	57.481	1.00	7.43	C
	ATOM 6966 C SER H 188	-2.977	37.694	57.665	1.00	6.97	C
	ATOM 6967 O SER H 188	-2.128	37.727	56.776	1.00	8.42	O
	ATOM 6968 CB SER H 188	-4.133	39.866	57.143	1.00	8.65	C
	ATOM 6969 OG SER H 188	-3.836	40.617	58.306	1.00	12.26	O
	ATOM 6970 N GLY H 189	-2.765	37.073	58.818	1.00	5.75	N
	ATOM 6971 CA GLY H 189	-1.511	36.395	59.063	1.00	3.96	C
	ATOM 6972 C GLY H 189	-0.463	37.311	59.648	1.00	5.18	C
	ATOM 6973 O GLY H 189	0.610	36.862	60.042	1.00	5.52	O
	ATOM 6974 N LEU H 190	-0.777	38.600	59.711	1.00	6.43	N
	ATOM 6975 CA LEU H 190	0.132	39.614	60.239	1.00	6.25	C
	ATOM 6976 C LEU H 190	-0.247	39.977	61.677	1.00	6.30	C
	ATOM 6977 O LEU H 190	-1.422	39.913	62.037	1.00	6.57	O
	ATOM 6978 CB LEU H 190	0.023	40.872	59.377	1.00	7.09	C
	ATOM 6979 CG LEU H 190	0.258	40.789	57.866	1.00	5.45	C
	ATOM 6980 CD1 LEU H 190	-0.363	41.995	57.184	1.00	2.55	C
	ATOM 6981 CD2 LEU H 190	1.745	40.694	57.578	1.00	5.29	C
	ATOM 6982 N TYR H 191	0.726	40.385	62.489	1.00	8.66	N
	ATOM 6983 CA TYR H 191	0.444	40.772	63.880	1.00	10.43	C
	ATOM 6984 C TYR H 191	0.209	42.274	64.038	1.00	11.98	C
	ATOM 6985 O TYR H 191	0.459	43.062	63.124	1.00	12.48	O
	ATOM 6986 CB TYR H 191	1.581	40.371	64.820	1.00	10.83	C
	ATOM 6987 CG TYR H 191	1.822	38.890	64.959	1.00	11.84	C
	ATOM 6988 CD1 TYR H 191	1.091	38.120	65.858	1.00	12.41	C
	ATOM 6989 CD2 TYR H 191	2.820	38.267	64.226	1.00	13.05	C
	ATOM 6990 CE1 TYR H 191	1.362	36.767	66.026	1.00	11.97	C
	ATOM 6991 CE2 TYR H 191	2.005	36.024	64.383	1.00	12.22	C

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FIG. 53-107	ATOM 6993 OH TYR H 191	2.690	34.852	65.455	1.00	13.42	O
	ATOM 6994 N SER H 192	-0.202	42.662	65.237	1.00	14.02	N
	ATOM 6995 CA SER H 192	-0.475	44.052	65.563	1.00	14.64	C
	ATOM 6996 C SER H 192	-0.597	44.200	67.088	1.00	15.31	C
	ATOM 6997 O SER H 192	-1.139	43.313	67.758	1.00	15.02	O
	ATOM 6998 CB SER H 192	-1.785	44.467	64.889	1.00	14.74	C
	ATOM 6999 OG SER H 192	-2.113	45.824	65.137	1.00	16.74	O
	ATOM 7000 N LEU H 193	-0.066	45.295	67.632	1.00	15.60	N
	ATOM 7001 CA LEU H 193	-0.142	45.569	69.075	1.00	15.39	C
	ATOM 7002 C LEU H 193	-0.047	47.077	69.316	1.00	15.95	C
	ATOM 7003 O LEU H 193	0.371	47.834	68.425	1.00	14.03	O
	ATOM 7004 CB LEU H 193	0.984	44.865	69.850	1.00	13.89	C
	ATOM 7005 CG LEU H 193	2.386	45.477	69.756	1.00	12.32	C
	ATOM 7006 CD1 LEU H 193	3.292	44.932	70.827	1.00	11.49	C
	ATOM 7007 CD2 LEU H 193	2.979	45.215	68.391	1.00	14.57	C
	ATOM 7008 N SER H 194	-0.415	47.502	70.522	1.00	15.26	N
	ATOM 7009 CA SER H 194	-0.375	48.911	70.889	1.00	15.50	C
	ATOM 7010 C SER H 194	0.456	49.149	72.141	1.00	14.88	C
	ATOM 7011 O SER H 194	0.453	48.343	73.081	1.00	14.55	O
	ATOM 7012 CB SER H 194	-1.793	49.456	71.118	1.00	15.26	C
	ATOM 7013 OG SER H 194	-2.572	49.370	69.940	1.00	16.76	O
	ATOM 7014 N SER H 195	1.180	50.259	72.135	1.00	14.05	N
	ATOM 7015 CA SER H 195	2.001	50.649	73.261	1.00	14.24	C
	ATOM 7016 C SER H 195	1.432	52.002	73.664	1.00	14.14	C
	ATOM 7017 O SER H 195	1.392	52.928	72.850	1.00	15.25	O
	ATOM 7018 CB SER H 195	3.467	50.773	72.832	1.00	14.96	C
	ATOM 7019 OG SER H 195	4.326	51.016	73.938	1.00	17.50	O
	ATOM 7020 N VAL H 196	0.923	52.087	74.888	1.00	13.38	N
	ATOM 7021 CA VAL H 196	0.327	53.313	75.399	1.00	12.73	C
	ATOM 7022 C VAL H 196	0.981	53.782	76.689	1.00	13.33	C
	ATOM 7023 O VAL H 196	1.380	52.975	77.517	1.00	12.87	O
	ATOM 7024 CB VAL H 196	-1.182	53.146	75.652	1.00	10.44	C
	ATOM 7025 CG1 VAL H 196	-1.889	52.794	74.354	1.00	5.83	C
	ATOM 7026 CG2 VAL H 196	-1.428	52.102	76.735	1.00	8.37	C
	ATOM 7027 N VAL H 197	1.102	55.097	76.834	1.00	14.77	N
	ATOM 7028 CA VAL H 197	1.700	55.707	78.014	1.00	15.10	C
	ATOM 7029 C VAL H 197	0.783	56.824	78.482	1.00	15.44	C
	ATOM 7030 O VAL H 197	0.309	57.632	77.682	1.00	14.98	O
	ATOM 7031 CB VAL H 197	3.130	56.261	77.725	1.00	15.42	C
	ATOM 7032 CG1 VAL H 197	3.111	57.210	76.547	1.00	15.39	C
	ATOM 7033 CG2 VAL H 197	3.709	56.938	78.965	1.00	15.02	C
	ATOM 7034 N THR H 198	0.465	56.802	79.768	1.00	16.66	N
	ATOM 7035 CA THR H 198	-0.398	57.794	80.358	1.00	19.74	C
	ATOM 7036 C THR H 198	0.461	58.898	80.955	1.00	22.76	C
	ATOM 7037 O THR H 198	1.408	58.632	81.692	1.00	25.76	O
	ATOM 7038 CB THR H 198	-1.289	57.161	81.426	1.00	19.71	C
	ATOM 7039 OG1 THR H 198	-0.484	56.422	82.354	1.00	21.22	O
	ATOM 7040 CG2 THR H 198	-2.286	56.214	80.773	1.00	22.04	C
	ATOM 7041 N VAL H 199	0.150	60.137	80.612	1.00	23.28	N
	ATOM 7042 CA VAL H 199	0.910	61.271	81.096	1.00	24.42	C
	ATOM 7043 C VAL H 199	-0.061	62.386	81.446	1.00	27.05	C
	ATOM 7044 O VAL H 199	-1.167	62.431	80.904	1.00	26.19	O
	ATOM 7045 CB VAL H 199	1.918	61.766	80.019	1.00	23.66	C
	ATOM 7046 CG1 VAL H 199	3.062	60.785	79.886	1.00	23.42	C
	ATOM 7047 CG2 VAL H 199	1.227	61.944	78.671	1.00	20.39	C
	ATOM 7048 N PRO H 200	0.305	63.255	82.413	1.00	28.35	N
	ATOM 7049 CA PRO H 200	-0.574	64.357	82.804	1.00	28.32	C
	ATOM 7050 C PRO H 200	-0.874	65.244	81.613	1.00	28.33	C
	ATOM 7051 O PRO H 200	-0.023	65.424	80.738	1.00	27.57	O
	ATOM 7052 CB PRO H 200	0.249	65.090	83.866	1.00	28.33	C
	ATOM 7053 CG PRO H 200	1.656	64.759	83.517	1.00	28.29	C
	ATOM 7054 CD PRO H 200	1.557	63.300	83.187	1.00	29.22	C
	ATOM 7055 N SER H 201	-2.091	65.776	81.578	1.00	29.98	N
	ATOM 7056 CA SER H 201	-2.551	66.652	80.500	1.00	31.65	C
	ATOM 7057 C SER H 201	-1.697	67.918	80.328	1.00	32.66	C
	ATOM 7058 O SER H 201	-1.690	68.541	79.265	1.00	31.83	O
	ATOM 7059 CB SER H 201	-4.005	67.052	80.762	1.00	32.43	C
	ATOM 7060 OG SER H 201	-4.777	65.936	81.176	1.00	32.44	O
	ATOM 7061 N SER H 202	-0.983	68.283	81.387	1.00	34.02	N
	ATOM 7062 CA SER H 202	-0.126	69.460	81.401	1.00	35.50	C

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FIG. 53-108

ATOM 7064	O	SER H 202	1.696	70.292	80.088	1.00	36.22	O
ATOM 7065	CB	SER H 202	0.165	69.844	82.850	1.00	36.50	C
ATOM 7066	OG	SER H 202	0.318	68.681	83.651	1.00	38.01	O
ATOM 7067	N	SER H 203	1.737	68.105	80.597	1.00	36.04	N
ATOM 7068	CA	SER H 203	2.997	67.854	79.898	1.00	35.59	C
ATOM 7069	C	SER H 203	2.866	68.019	78.389	1.00	35.77	C
ATOM 7070	O	SER H 203	3.743	68.590	77.731	1.00	37.10	O
ATOM 7071	CB	SER H 203	3.511	66.449	80.216	1.00	34.75	C
ATOM 7072	OG	SER H 203	3.809	66.309	81.597	1.00	36.94	O
ATOM 7073	N	LEU H 204	1.763	67.518	77.846	1.00	34.93	N
ATOM 7074	CA	LEU H 204	1.498	67.584	76.418	1.00	34.76	C
ATOM 7075	C	LEU H 204	1.857	68.962	75.865	1.00	35.53	C
ATOM 7076	O	LEU H 204	1.592	69.990	76.496	1.00	36.23	O
ATOM 7077	CB	LEU H 204	0.023	67.282	76.156	1.00	33.94	C
ATOM 7078	CG	LEU H 204	-0.537	66.058	76.892	1.00	34.12	C
ATOM 7079	CD1	LEU H 204	-2.018	65.881	76.600	1.00	32.48	C
ATOM 7080	CD2	LEU H 204	0.243	64.821	76.493	1.00	34.75	C
ATOM 7081	N	GLY H 205	2.465	68.985	74.688	1.00	35.90	N
ATOM 7082	CA	GLY H 205	2.856	70.251	74.099	1.00	36.54	C
ATOM 7083	C	GLY H 205	4.241	70.646	74.581	1.00	36.78	C
ATOM 7084	O	GLY H 205	5.156	70.809	73.771	1.00	37.69	O
ATOM 7085	N	THR H 206	4.404	70.790	75.894	1.00	35.10	N
ATOM 7086	CA	THR H 206	5.698	71.148	76.461	1.00	32.96	C
ATOM 7087	C	THR H 206	6.646	69.985	76.180	1.00	31.40	C
ATOM 7088	O	THR H 206	7.620	70.121	75.430	1.00	31.35	O
ATOM 7089	CB	THR H 206	5.609	71.339	77.981	1.00	32.63	C
ATOM 7090	OG1	THR H 206	4.294	71.778	78.339	1.00	33.03	O
ATOM 7091	CG2	THR H 206	6.613	72.379	78.433	1.00	34.20	C
ATOM 7092	N	GLN H 207	6.352	68.847	76.802	1.00	29.76	N
ATOM 7093	CA	GLN H 207	7.125	67.625	76.633	1.00	27.98	C
ATOM 7094	C	GLN H 207	6.445	66.797	75.552	1.00	28.19	C
ATOM 7095	O	GLN H 207	5.266	66.456	75.674	1.00	28.33	O
ATOM 7096	CB	GLN H 207	7.161	66.839	77.946	1.00	26.33	C
ATOM 7097	CG	GLN H 207	7.669	65.415	77.825	1.00	26.06	C
ATOM 7098	CD	GLN H 207	9.110	65.326	77.354	1.00	25.96	C
ATOM 7099	OE1	GLN H 207	9.438	65.706	76.225	1.00	25.74	O
ATOM 7100	NE2	GLN H 207	9.981	64.821	78.220	1.00	24.52	N
ATOM 7101	N	THR H 208	7.167	66.542	74.467	1.00	28.37	N
ATOM 7102	CA	THR H 208	6.642	65.752	73.355	1.00	27.66	C
ATOM 7103	C	THR H 208	6.928	64.277	73.646	1.00	27.73	C
ATOM 7104	O	THR H 208	7.574	63.952	74.647	1.00	29.05	O
ATOM 7105	CB	THR H 208	7.276	66.182	72.006	1.00	27.09	C
ATOM 7106	OG1	THR H 208	8.658	65.799	71.961	1.00	26.14	O
ATOM 7107	CG2	THR H 208	7.184	67.696	71.834	1.00	25.02	C
ATOM 7108	N	TYR H 209	6.455	63.381	72.791	1.00	26.40	N
ATOM 7109	CA	TYR H 209	6.666	61.956	73.026	1.00	25.94	C
ATOM 7110	C	TYR H 209	6.940	61.150	71.770	1.00	25.67	C
ATOM 7111	O	TYR H 209	6.332	61.382	70.725	1.00	23.61	O
ATOM 7112	CB	TYR H 209	5.477	61.366	73.785	1.00	24.52	C
ATOM 7113	CG	TYR H 209	5.357	61.911	75.181	1.00	25.18	C
ATOM 7114	CD1	TYR H 209	6.143	61.402	76.210	1.00	25.69	C
ATOM 7115	CD2	TYR H 209	4.492	62.967	75.468	1.00	24.68	C
ATOM 7116	CE1	TYR H 209	6.080	61.926	77.493	1.00	27.59	C
ATOM 7117	CE2	TYR H 209	4.418	63.502	76.750	1.00	27.78	C
ATOM 7118	CZ	TYR H 209	5.216	62.977	77.760	1.00	28.92	C
ATOM 7119	OH	TYR H 209	5.168	63.507	79.034	1.00	30.88	O
ATOM 7120	N	ILE H 210	7.844	60.183	71.892	1.00	26.57	N
ATOM 7121	CA	ILE H 210	8.219	59.342	70.764	1.00	28.79	C
ATOM 7122	C	ILE H 210	8.228	57.863	71.134	1.00	28.99	C
ATOM 7123	O	ILE H 210	8.675	57.492	72.224	1.00	28.57	O
ATOM 7124	CB	ILE H 210	9.631	59.697	70.253	1.00	29.02	C
ATOM 7125	CG1	ILE H 210	9.696	61.169	69.845	1.00	29.17	C
ATOM 7126	CG2	ILE H 210	10.011	58.787	69.084	1.00	28.88	C
ATOM 7127	CD1	ILE H 210	11.100	61.672	69.602	1.00	28.35	C
ATOM 7128	N	CYSH 211	7.705	57.030	70.236	1.00	29.45	N
ATOM 7129	CA	CYSH 211	7.703	55.584	70.449	1.00	29.08	C
ATOM 7130	C	CYSH 211	8.668	54.952	69.438	1.00	28.27	C
ATOM 7131	O	CYSH 211	8.516	55.106	68.223	1.00	27.49	O
ATOM 7132	CB	CYSH 211	6.301	54.986	70.296	1.00	27.46	C
ATOM 7133	CG	CYSH 211	5.745	54.792	69.581	1.00	26.97	C

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FIG. 53-109	ATOM 7135 CA ASN H 212	10.712	53.667	69.120	1.00	25.61	C
	ATOM 7136 C ASN H 212	10.248	52.238	68.890	1.00	23.30	C
	ATOM 7137 O ASN H 212	10.024	51.495	69.844	1.00	22.85	O
	ATOM 7138 CB ASN H 212	12.062	53.698	69.828	1.00	27.19	C
	ATOM 7139 CG ASN H 212	12.313	55.016	70.536	1.00	28.04	C
	ATOM 7140 OD1 ASN H 212	12.541	55.051	71.752	1.00	28.39	O
	ATOM 7141 ND2 ASN H 212	12.235	56.112	69.792	1.00	27.04	N
	ATOM 7142 N VAL H 213	10.053	51.881	67.627	1.00	21.53	N
	ATOM 7143 CA VAL H 213	9.582	50.553	67.248	1.00	20.85	C
	ATOM 7144 C VAL H 213	10.627	49.769	66.460	1.00	19.23	C
	ATOM 7145 O VAL H 213	10.848	50.030	65.281	1.00	18.38	O
	ATOM 7146 CB VAL H 213	8.303	50.662	66.411	1.00	21.35	C
	ATOM 7147 CG1 VAL H 213	7.799	49.279	66.026	1.00	21.26	C
	ATOM 7148 CG2 VAL H 213	7.249	51.447	67.181	1.00	20.95	C
	ATOM 7149 N ASN H 214	11.277	48.817	67.114	1.00	19.12	N
	ATOM 7150 CA ASN H 214	12.304	48.021	66.447	1.00	19.03	C
	ATOM 7151 C ASN H 214	11.766	46.667	66.013	1.00	17.33	C
	ATOM 7152 O ASN H 214	10.867	46.098	66.638	1.00	14.41	O
	ATOM 7153 CB ASN H 214	13.527	47.837	67.353	1.00	21.24	C
	ATOM 7154 CG ASN H 214	14.671	47.096	66.665	1.00	22.32	C
	ATOM 7155 OD1 ASN H 214	15.508	47.701	65.997	1.00	22.05	O
	ATOM 7156 ND2 ASN H 214	14.733	45.787	66.863	1.00	23.88	N
	ATOM 7157 N HIS H 215	12.340	46.157	64.934	1.00	17.25	N
	ATOM 7158 CA HIS H 215	11.954	44.879	64.381	1.00	16.34	C
	ATOM 7159 C HIS H 215	13.189	44.329	63.672	1.00	17.87	C
	ATOM 7160 O HIS H 215	13.558	44.796	62.597	1.00	18.68	O
	ATOM 7161 CB HIS H 215	10.814	45.071	63.386	1.00	13.92	C
	ATOM 7162 CG HIS H 215	10.074	43.812	63.062	1.00	12.54	C
	ATOM 7163 ND1 HIS H 215	9.309	43.668	61.930	1.00	14.48	N
	ATOM 7164 CD2 HIS H 215	9.968	42.642	63.740	1.00	12.09	C
	ATOM 7165 CE1 HIS H 215	8.755	42.471	61.919	1.00	12.28	C
	ATOM 7166 NE2 HIS H 215	9.140	41.828	63.010	1.00	11.26	N
	ATOM 7167 N LYS H 216	13.852	43.367	64.300	1.00	19.14	N
	ATOM 7168 CA LYS H 216	15.038	42.761	63.726	1.00	21.68	C
	ATOM 7169 C LYS H 216	14.739	41.988	62.435	1.00	22.97	C
	ATOM 7170 O LYS H 216	15.407	42.187	61.417	1.00	22.37	O
	ATOM 7171 CB LYS H 216	15.691	41.834	64.750	1.00	24.90	C
	ATOM 7172 CG LYS H 216	17.172	41.612	64.539	1.00	30.77	C
	ATOM 7173 CD LYS H 216	17.978	42.274	65.654	1.00	36.75	C
	ATOM 7174 CE LYS H 216	17.728	43.785	65.754	1.00	40.46	C
	ATOM 7175 NZ LYS H 216	18.392	44.376	66.961	1.00	41.89	N
	ATOM 7176 N PRO H 217	13.699	41.128	62.440	1.00	23.59	N
	ATOM 7177 CA PRO H 217	13.375	40.358	61.234	1.00	23.65	C
	ATOM 7178 C PRO H 217	13.316	41.168	59.944	1.00	24.82	C
	ATOM 7179 O PRO H 217	13.583	40.637	58.861	1.00	26.99	O
	ATOM 7180 CB PRO H 217	12.021	39.754	61.578	1.00	22.68	C
	ATOM 7181 CG PRO H 217	12.155	39.488	63.032	1.00	22.06	C
	ATOM 7182 CD PRO H 217	12.763	40.781	63.527	1.00	23.22	C
	ATOM 7183 N SER H 218	12.974	42.448	60.050	1.00	24.15	N
	ATOM 7184 CA SER H 218	12.874	43.288	58.861	1.00	23.21	C
	ATOM 7185 C SER H 218	13.905	44.412	58.831	1.00	25.33	C
	ATOM 7186 O SER H 218	13.905	45.235	57.904	1.00	25.52	O
	ATOM 7187 CB SER H 218	11.461	43.862	58.752	1.00	17.61	C
	ATOM 7188 OG SER H 218	11.070	44.463	59.971	1.00	10.47	O
	ATOM 7189 N ASN H 219	14.811	44.409	59.812	1.00	26.07	N
	ATOM 7190 CA ASN H 219	15.826	45.448	59.928	1.00	25.29	C
	ATOM 7191 C ASN H 219	15.117	46.793	59.950	1.00	23.66	C
	ATOM 7192 O ASN H 219	15.470	47.714	59.219	1.00	22.34	O
	ATOM 7193 CB ASN H 219	16.799	45.383	58.755	1.00	28.99	C
	ATOM 7194 CG ASN H 219	18.008	44.531	59.051	1.00	30.63	C
	ATOM 7195 OD1 ASN H 219	17.883	43.369	59.422	1.00	31.67	O
	ATOM 7196 ND2 ASN H 219	19.193	45.106	58.888	1.00	32.29	N
	ATOM 7197 N THR H 220	14.084	46.870	60.775	1.00	22.97	N
	ATOM 7198 CA THR H 220	13.286	48.066	60.907	1.00	23.30	C
	ATOM 7199 C THR H 220	13.308	48.621	62.322	1.00	24.58	C
	ATOM 7200 O THR H 220	13.240	47.882	63.312	1.00	23.13	O
	ATOM 7201 CB THR H 220	11.805	47.805	60.526	1.00	21.35	C
	ATOM 7202 OG1 THR H 220	11.733	47.337	59.180	1.00	21.56	O
	ATOM 7203 CG2 THR H 220	10.976	49.068	60.638	1.00	21.72	C
	ATOM 7204 N LYS H 221	12.426	40.841	62.381	1.00	26.22	N

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FIG. 53-110	ATOM 7206 C LYS H 221	12.739	51.993	63.162	1.00	26.45	C
	ATOM 7207 O LYS H 221	13.098	52.556	62.127	1.00	26.86	O
	ATOM 7208 CB LYS H 221	14.816	50.988	64.151	1.00	25.28	C
	ATOM 7209 CG LYS H 221	14.777	51.554	65.556	1.00	26.33	C
	ATOM 7210 CD LYS H 221	16.133	51.589	66.222	1.00	28.37	C
	ATOM 7211 CE LYS H 221	16.033	52.340	67.539	1.00	29.82	C
	ATOM 7212 NZ LYS H 221	17.288	52.295	68.330	1.00	29.18	N
	ATOM 7213 N VAL H 222	11.692	52.384	63.870	1.00	26.93	N
	ATOM 7214 CA VAL H 222	10.946	53.579	63.524	1.00	28.68	C
	ATOM 7215 C VAL H 222	10.596	54.378	64.770	1.00	29.43	C
	ATOM 7216 O VAL H 222	10.227	53.815	65.798	1.00	29.62	O
	ATOM 7217 CB VAL H 222	9.624	53.210	62.819	1.00	29.88	C
	ATOM 7218 CG1 VAL H 222	8.837	54.465	62.460	1.00	29.69	C
	ATOM 7219 CG2 VAL H 222	9.896	52.356	61.598	1.00	29.32	C
	ATOM 7220 N ASP H 223	10.697	55.693	64.670	1.00	31.29	N
	ATOM 7221 CA ASP H 223	10.362	56.567	65.784	1.00	31.74	C
	ATOM 7222 C ASP H 223	9.114	57.323	65.316	1.00	31.35	C
	ATOM 7223 O ASP H 223	8.960	57.595	64.125	1.00	30.17	O
	ATOM 7224 CB ASP H 223	11.531	57.519	66.073	1.00	32.60	C
	ATOM 7225 CG ASP H 223	12.876	56.792	66.178	1.00	31.98	C
	ATOM 7226 OD1 ASP H 223	13.230	56.319	67.280	1.00	29.31	O
	ATOM 7227 OD2 ASP H 223	13.580	56.699	65.149	1.00	32.64	O
	ATOM 7228 N LYS H 224	8.198	57.602	66.234	1.00	31.93	N
	ATOM 7229 CA LYS H 224	6.964	58.291	65.883	1.00	34.40	C
	ATOM 7230 C LYS H 224	6.479	59.180	67.021	1.00	36.63	C
	ATOM 7231 O LYS H 224	6.118	58.690	68.101	1.00	35.77	O
	ATOM 7232 CB LYS H 224	5.880	57.267	65.535	1.00	35.25	C
	ATOM 7233 CG LYS H 224	4.519	57.856	65.198	1.00	35.97	C
	ATOM 7234 CD LYS H 224	4.544	58.580	63.863	1.00	38.19	C
	ATOM 7235 CE LYS H 224	3.171	59.133	63.515	1.00	39.84	C
	ATOM 7236 NZ LYS H 224	3.031	59.588	62.104	1.00	39.10	N
	ATOM 7237 N LYS H 225	6.497	60.489	66.781	1.00	38.47	N
	ATOM 7238 CA LYS H 225	6.047	61.450	67.777	1.00	40.00	C
	ATOM 7239 C LYS H 225	4.532	61.513	67.761	1.00	40.56	C
	ATOM 7240 O LYS H 225	3.919	61.593	66.690	1.00	40.71	O
	ATOM 7241 CB LYS H 225	6.627	62.842	67.512	1.00	41.38	C
	ATOM 7242 CG LYS H 225	6.069	63.928	68.438	1.00	43.12	C
	ATOM 7243 CD LYS H 225	6.731	65.280	68.225	1.00	44.83	C
	ATOM 7244 CE LYS H 225	8.227	65.214	68.501	1.00	46.17	C
	ATOM 7245 NZ LYS H 225	8.872	66.552	68.416	1.00	47.79	N
	ATOM 7246 N VAL H 226	3.937	61.450	68.946	1.00	41.43	N
	ATOM 7247 CA VAL H 226	2.490	61.514	69.071	1.00	42.84	C
	ATOM 7248 C VAL H 226	2.073	62.974	69.216	1.00	44.17	C
	ATOM 7249 O VAL H 226	2.381	63.628	70.218	1.00	43.46	O
	ATOM 7250 CB VAL H 226	1.979	60.701	70.279	1.00	41.78	C
	ATOM 7251 CG1 VAL H 226	0.472	60.507	70.172	1.00	40.41	C
	ATOM 7252 CG2 VAL H 226	2.687	59.358	70.353	1.00	40.96	C
	ATOM 7253 N GLU H 227	1.435	63.494	68.176	1.00	45.83	N
	ATOM 7254 CA GLU H 227	0.971	64.873	68.156	1.00	46.70	C
	ATOM 7255 C GLU H 227	-0.179	65.042	69.132	1.00	47.48	C
	ATOM 7256 O GLU H 227	-1.005	64.151	69.290	1.00	48.42	O
	ATOM 7257 CB GLU H 227	0.557	65.306	66.733	1.00	46.15	C
	ATOM 7258 CG GLU H 227	-0.282	64.301	65.931	1.00	45.39	C
	ATOM 7259 CD GLU H 227	0.547	63.185	65.312	1.00	44.09	C
	ATOM 7260 OE1 GLU H 227	1.155	63.402	64.243	1.00	44.02	O
	ATOM 7261 OE2 GLU H 227	0.584	62.084	65.894	1.00	42.58	O
	ATOM 7262 N PRO H 228	-0.237	66.186	69.817	1.00	48.64	N
	ATOM 7263 CA PRO H 228	-1.297	66.463	70.790	1.00	49.52	C
	ATOM 7264 C PRO H 228	-2.695	66.664	70.210	1.00	49.89	C
	ATOM 7265 O PRO H 228	-2.855	67.026	69.044	1.00	48.97	O
	ATOM 7266 CB PRO H 228	-0.793	67.721	71.482	1.00	50.46	C
	ATOM 7267 CG PRO H 228	-0.054	68.421	70.378	1.00	50.48	C
	ATOM 7268 CD PRO H 228	0.722	67.300	69.750	1.00	49.24	C
	ATOM 7269 N LYS H 229	-3.696	66.420	71.055	1.00	51.01	N
	ATOM 7270 CA LYS H 229	-5.109	66.571	70.708	1.00	50.89	C
	ATOM 7271 C LYS H 229	-5.964	66.499	71.975	1.00	49.93	C
	ATOM 7272 O LYS H 229	-6.378	67.582	72.444	1.00	49.29	O
	ATOM 7273 CB LYS H 229	-5.560	65.494	69.710	1.00	50.99	C
	ATOM 7274 CG LYS H 229	-7.049	65.559	69.333	1.00	51.00	C

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FIG. 53-111	ATOM 7277 NZ LYSH 229	-8.352	68.958	70.228	1.00	54.11	N
	TER 7278 LYSH 229						
	HETATM 7279 O HOH 1	22.165	9.529	79.160	1.00	2.00	O
	HETATM 7280 O HOH 2	11.911	1.801	70.392	1.00	6.27	O
	HETATM 7281 O HOH 3	1.103	23.950	73.530	1.00	2.00	O
	HETATM 7282 O HOH 4	13.339	9.604	88.234	1.00	2.00	O
	HETATM 7283 O HOH 5	32.518	-17.948	103.755	1.00	4.10	O
	HETATM 7284 O HOH 6	-25.644	45.440	74.531	1.00	2.00	O
	HETATM 7285 O HOH 7	50.290	18.960	56.862	1.00	2.00	O
	HETATM 7286 O HOH 8	38.873	-2.572	84.241	1.00	2.00	O
	HETATM 7287 O HOH 9	22.766	-42.838	87.811	1.00	4.05	O
	HETATM 7288 O HOH 10	27.297	-7.705	74.948	1.00	2.00	O
	HETATM 7289 O HOH 11	-2.591	36.529	85.413	1.00	2.00	O
	HETATM 7290 O HOH 12	-10.145	19.754	92.343	1.00	2.00	O
	HETATM 7291 O HOH 13	14.134	-5.783	94.278	1.00	2.00	O
	HETATM 7292 O HOH 14	16.122	23.074	97.779	1.00	2.00	O
	HETATM 7293 O HOH 15	17.049	-42.606	77.879	1.00	2.05	O
	HETATM 7294 O HOH 16	37.979	-6.682	96.642	1.00	2.00	O
	HETATM 7295 O HOH 17	-2.446	25.504	77.697	1.00	2.00	O
	HETATM 7296 O HOH 18	19.949	4.273	89.649	1.00	2.13	O
	HETATM 7297 O HOH 19	15.645	5.014	68.450	1.00	2.00	O
	HETATM 7298 O HOH 20	-19.962	42.751	63.628	1.00	2.92	O
	HETATM 7299 O HOH 21	59.945	-15.290	74.664	1.00	2.14	O
	HETATM 7300 O HOH 22	10.277	61.569	79.315	1.00	2.97	O
	HETATM 7301 O HOH 23	-9.504	39.045	92.132	1.00	4.39	O
	HETATM 7302 O HOH 24	-1.295	32.363	59.813	1.00	6.79	O
	HETATM 7303 O HOH 25	-10.346	15.142	92.580	1.00	5.85	O
	HETATM 7304 O HOH 26	43.551	-12.354	97.257	1.00	2.00	O
	HETATM 7305 O HOH 27	59.784	28.541	67.004	1.00	8.19	O
	HETATM 7306 O HOH 28	7.111	18.959	100.259	1.00	3.59	O
	HETATM 7307 O HOH 29	14.885	-24.670	80.511	1.00	8.88	O
	HETATM 7308 O HOH 30	-2.619	64.345	85.123	1.00	2.00	O
	HETATM 7309 O HOH 31	37.275	-15.380	109.070	1.00	2.00	O
	HETATM 7310 O HOH 32	23.327	-9.758	81.087	1.00	5.64	O
	HETATM 7311 O HOH 33	41.146	-13.975	83.133	1.00	8.88	O
	HETATM 7312 O HOH 34	-5.559	35.837	106.706	1.00	2.00	O
	HETATM 7313 O HOH 35	39.858	-31.312	80.857	1.00	2.62	O
	HETATM 7314 O HOH 36	-6.964	34.744	99.440	1.00	6.18	O
	HETATM 7315 O HOH 37	8.406	56.401	59.861	1.00	14.11	O
	HETATM 7316 O HOH 38	28.098	-17.419	68.859	1.00	9.36	O
	HETATM 7317 O HOH 39	7.309	32.808	56.517	1.00	3.40	O
	HETATM 7318 O HOH 40	48.182	18.003	55.687	1.00	5.31	O
	HETATM 7319 O HOH 41	13.560	8.574	76.389	1.00	3.44	O
	HETATM 7320 O HOH 42	44.794	-32.062	86.982	1.00	2.00	O
	HETATM 7321 O HOH 43	3.416	46.935	81.161	1.00	3.06	O
	HETATM 7322 O HOH 44	9.905	58.282	61.578	1.00	6.16	O
	HETATM 7323 O HOH 45	3.954	66.270	66.601	1.00	2.00	O
	HETATM 7324 O HOH 46	34.782	-30.843	80.859	1.00	2.00	O
	HETATM 7325 O HOH 47	6.378	71.557	81.908	1.00	5.92	O
	HETATM 7326 O HOH 48	-10.103	62.639	59.099	1.00	6.28	O
	HETATM 7327 O HOH 49	57.029	-8.449	52.647	1.00	9.33	O
	HETATM 7328 O HOH 50	12.704	-24.369	84.770	1.00	6.18	O
	HETATM 7329 O HOH 51	17.676	15.222	63.164	1.00	3.84	O
	HETATM 7330 O HOH 52	54.823	-7.050	50.766	1.00	2.00	O
	HETATM 7331 O HOH 53	42.016	-32.002	82.471	1.00	2.00	O
	HETATM 7332 O HOH 54	-1.192	9.535	72.350	1.00	7.59	O
	HETATM 7333 O HOH 55	60.614	10.882	65.751	1.00	4.69	O
	HETATM 7334 O HOH 56	4.080	59.007	82.151	1.00	4.10	O
	HETATM 7335 O HOH 57	46.087	-28.223	99.118	1.00	4.68	O
	HETATM 7336 O HOH 58	0.678	37.773	54.674	1.00	2.55	O
	HETATM 7337 O HOH 59	11.861	-0.136	83.796	1.00	2.56	O
	HETATM 7338 O HOH 60	-0.333	44.117	95.564	1.00	10.62	O
	HETATM 7339 O HOH 61	27.052	-12.944	69.452	1.00	7.64	O
	HETATM 7340 O HOH 62	-2.539	47.008	94.502	1.00	12.92	O
	HETATM 7341 O HOH 63	36.964	-23.164	76.315	1.00	4.23	O
	HETATM 7342 O HOH 64	49.693	-12.767	79.396	1.00	8.13	O
	HETATM 7343 O HOH 65	15.462	15.223	80.328	1.00	10.92	O
	HETATM 7344 O HOH 66	62.573	-4.720	59.499	1.00	10.84	O
	HETATM 7345 O HOH 67	5.569	58.370	89.372	1.00	9.52	O
	HETATM 7346 O HOH 68	7.460	43.460	65.953	1.00	9.47	O



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FIG. 53-112

HETATM 7348	O	HOH	70	7.955	0.339	72.229	1.00	8.67	O
HETATM 7349	O	HOH	71	14.698	51.000	59.877	1.00	7.66	O
HETATM 7350	O	HOH	72	60.442	14.789	68.692	1.00	13.94	O
HETATM 7351	O	HOH	73	29.550	5.626	76.429	1.00	9.44	O
HETATM 7352	O	HOH	74	23.488	-12.795	103.491	1.00	7.66	O
HETATM 7353	O	HOH	75	55.350	-17.876	76.419	1.00	11.30	O
HETATM 7354	O	HOH	76	-3.980	55.107	64.298	1.00	7.49	O
HETATM 7355	O	HOH	77	31.336	-37.543	88.786	1.00	12.45	O
HETATM 7356	O	HOH	78	53.764	13.270	60.229	1.00	7.00	O
HETATM 7357	O	HOH	79	22.510	-14.728	88.570	1.00	13.52	O
HETATM 7358	O	HOH	80	26.954	18.767	65.939	1.00	10.42	O
HETATM 7359	O	HOH	81	17.435	-24.103	93.619	1.00	11.09	O
HETATM 7360	O	HOH	82	2.324	16.962	77.639	1.00	11.45	O
HETATM 7361	O	HOH	83	42.819	-10.854	76.734	1.00	12.42	O
HETATM 7362	O	HOH	84	19.836	-2.530	99.533	1.00	12.41	O
HETATM 7363	O	HOH	85	17.370	-13.308	101.942	1.00	8.42	O
HETATM 7364	O	HOH	86	11.146	66.878	74.135	1.00	12.89	O
HETATM 7365	O	HOH	87	39.173	-24.013	77.444	1.00	7.92	O
HETATM 7366	O	HOH	88	14.477	24.016	86.336	1.00	10.87	O
HETATM 7367	O	HOH	89	68.983	35.023	53.834	1.00	15.42	O
HETATM 7368	O	HOH	90	66.303	-5.484	68.312	1.00	8.44	O
HETATM 7369	O	HOH	91	69.207	8.623	48.984	1.00	3.58	O
HETATM 7370	O	HOH	92	15.670	1.312	76.211	1.00	7.75	O
HETATM 7371	O	HOH	93	50.357	15.548	50.843	1.00	7.95	O
HETATM 7372	O	HOH	94	-12.212	65.127	77.508	1.00	11.88	O
HETATM 7373	O	HOH	95	10.631	32.727	91.432	1.00	13.61	O
HETATM 7374	O	HOH	96	9.439	9.433	64.343	1.00	13.19	O
HETATM 7375	O	HOH	97	24.875	-30.408	73.942	1.00	6.08	O
HETATM 7376	O	HOH	98	6.838	41.588	69.878	1.00	16.99	O
HETATM 7377	O	HOH	99	13.587	31.324	95.823	1.00	7.70	O
HETATM 7378	O	HOH	100	44.463	-29.489	74.048	1.00	2.00	O
HETATM 7379	O	HOH	101	51.342	1.341	76.032	1.00	10.66	O
HETATM 7380	O	HOH	102	51.212	-28.609	69.751	1.00	16.76	O
HETATM 7381	O	HOH	103	5.423	47.471	55.773	1.00	9.10	O
HETATM 7382	O	HOH	104	-3.178	38.328	73.176	1.00	15.56	O
HETATM 7383	O	HOH	105	10.637	53.193	76.911	1.00	12.15	O
HETATM 7384	O	HOH	106	22.795	-12.364	86.133	1.00	18.01	O
HETATM 7385	O	HOH	107	27.091	-22.792	106.177	1.00	10.59	O
HETATM 7386	O	HOH	108	15.923	23.867	90.058	1.00	13.78	O
HETATM 7387	O	HOH	109	-9.008	13.858	77.706	1.00	8.30	O
HETATM 7388	O	HOH	110	3.704	57.214	61.407	1.00	11.60	O
HETATM 7389	O	HOH	111	-3.669	43.253	55.419	1.00	16.77	O
HETATM 7390	O	HOH	112	33.501	-1.832	86.297	1.00	11.89	O
HETATM 7391	O	HOH	113	42.661	-26.173	71.459	1.00	20.46	O
HETATM 7392	O	HOH	114	31.043	17.252	64.838	1.00	15.53	O
HETATM 7393	O	HOH	115	-4.504	34.542	84.856	1.00	9.88	O
HETATM 7394	O	HOH	116	53.047	23.643	46.970	1.00	10.95	O
HETATM 7395	O	HOH	117	16.022	-19.990	86.523	1.00	15.78	O
HETATM 7396	O	HOH	118	20.590	28.045	81.230	1.00	9.39	O
HETATM 7397	O	HOH	119	48.277	-6.022	83.992	1.00	10.97	O
HETATM 7398	O	HOH	120	57.036	-24.902	98.133	1.00	16.18	O
HETATM 7399	O	HOH	121	5.591	52.123	58.678	1.00	12.13	O
HETATM 7400	O	HOH	122	0.961	35.324	86.508	1.00	15.96	O
HETATM 7401	O	HOH	123	35.507	-25.465	74.447	1.00	16.04	O
HETATM 7402	O	HOH	124	28.949	-14.394	76.841	1.00	11.40	O
HETATM 7403	O	HOH	125	-6.401	60.822	84.877	1.00	17.22	O
HETATM 7404	O	HOH	126	-0.337	46.472	83.468	1.00	11.84	O
HETATM 7405	O	HOH	127	-6.936	34.868	82.669	1.00	21.10	O
HETATM 7406	O	HOH	128	70.351	32.466	57.167	1.00	16.84	O
HETATM 7407	O	HOH	129	42.235	-28.673	72.078	1.00	12.31	O
HETATM 7408	O	HOH	130	27.003	7.858	71.274	1.00	17.91	O
HETATM 7409	O	HOH	131	-20.266	54.933	52.694	1.00	9.75	O
HETATM 7410	O	HOH	132	-4.357	8.994	96.842	1.00	7.58	O
HETATM 7411	O	HOH	133	28.406	-16.947	76.829	1.00	13.90	O
HETATM 7412	O	HOH	134	8.543	58.475	83.123	1.00	10.11	O
HETATM 7413	O	HOH	135	18.494	12.809	61.570	1.00	15.24	O
HETATM 7414	O	HOH	136	28.075	-30.594	95.656	1.00	4.74	O
HETATM 7415	O	HOH	137	42.938	-45.127	78.791	1.00	17.56	O
HETATM 7416	O	HOH	138	28.751	-11.594	107.122	1.00	12.51	O
HETATM 7417	O	HOH	139	42.264	12.006	70.405	1.00	10.56	O

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FIG. 53-113	HETATM 7419	O	HOH	141	55.796	-20.368	75.764	1.00	10.04	O
	HETATM 7420	O	HOH	142	7.955	3.518	72.301	1.00	15.50	O
	HETATM 7421	O	HOH	143	5.388	7.280	69.370	1.00	13.93	O
	HETATM 7422	O	HOH	144	50.714	-0.970	55.913	1.00	12.13	O
	HETATM 7423	O	HOH	145	11.373	31.813	77.043	1.00	18.74	O
	HETATM 7424	O	HOH	146	10.609	65.109	80.839	1.00	15.07	O
	HETATM 7425	O	HOH	147	-22.776	48.048	84.973	1.00	13.08	O
	HETATM 7426	O	HOH	148	2.152	14.209	63.515	1.00	19.36	O
	HETATM 7427	O	HOH	149	28.677	-15.259	109.865	1.00	11.03	O
	HETATM 7428	O	HOH	150	55.391	19.247	46.436	1.00	11.06	O
	HETATM 7429	O	HOH	151	54.946	-11.772	89.245	1.00	22.22	O
	HETATM 7430	O	HOH	152	27.897	19.384	78.558	1.00	18.71	O
	HETATM 7431	O	HOH	153	-23.058	54.253	79.253	1.00	14.83	O
	HETATM 7432	O	HOH	154	29.804	25.684	81.988	1.00	17.86	O
	HETATM 7433	O	HOH	155	33.062	-0.846	92.984	1.00	8.46	O
	HETATM 7434	O	HOH	156	-10.657	11.384	84.281	1.00	12.49	O
	HETATM 7435	O	HOH	157	12.381	27.954	90.699	1.00	17.73	O
	HETATM 7436	O	HOH	158	13.676	44.432	68.890	1.00	11.16	O
	HETATM 7437	O	HOH	159	61.317	37.504	51.767	1.00	13.49	O
	HETATM 7438	O	HOH	160	17.791	18.137	95.261	1.00	14.35	O
	HETATM 7439	O	HOH	161	14.379	52.980	71.925	1.00	16.56	O
	HETATM 7440	O	HOH	162	41.192	-22.679	59.991	1.00	17.07	O
	HETATM 7441	O	HOH	163	48.359	-29.507	77.036	1.00	24.31	O
	HETATM 7442	O	HOH	164	43.551	-33.235	89.036	1.00	15.63	O
	HETATM 7443	O	HOH	165	-19.552	65.707	65.325	1.00	16.30	O
	HETATM 7444	O	HOH	166	51.766	-18.992	77.503	1.00	10.87	O
	HETATM 7445	O	HOH	167	-7.552	31.531	83.394	1.00	12.41	O
	HETATM 7446	O	HOH	168	70.680	23.618	50.621	1.00	10.11	O
	HETATM 7447	O	HOH	169	2.712	17.305	94.600	1.00	14.68	O
	HETATM 7448	O	HOH	170	24.298	-9.578	68.345	1.00	12.50	O
	HETATM 7449	O	HOH	171	0.246	5.938	74.609	1.00	14.87	O
	HETATM 7450	O	HOH	172	-5.220	44.555	69.546	1.00	13.80	O
	HETATM 7451	O	HOH	173	39.118	-24.386	61.724	1.00	8.70	O
	HETATM 7452	O	HOH	174	24.181	-9.027	64.624	1.00	13.71	O
	HETATM 7453	O	HOH	175	3.695	39.485	54.069	1.00	15.15	O
	HETATM 7454	O	HOH	176	17.117	52.940	61.036	1.00	13.69	O
	HETATM 7455	O	HOH	177	10.828	8.090	62.402	1.00	26.25	O
	HETATM 7456	O	HOH	178	32.268	-38.218	86.345	1.00	17.93	O
	HETATM 7457	O	HOH	179	73.798	27.825	52.191	1.00	24.74	O
	HETATM 7458	O	HOH	180	59.358	-4.565	64.787	1.00	15.43	O
	HETATM 7459	O	HOH	181	41.535	-2.375	86.744	1.00	7.10	O
	HETATM 7460	O	HOH	182	-8.946	29.518	82.336	1.00	15.69	O
	HETATM 7461	O	HOH	183	55.326	15.266	47.219	1.00	17.04	O
	HETATM 7462	O	HOH	184	29.904	-21.145	109.019	1.00	27.75	O
	HETATM 7463	O	HOH	185	2.643	2.395	80.292	1.00	12.45	O
	HETATM 7464	O	HOH	186	22.721	-1.471	50.919	1.00	20.96	O
	HETATM 7465	O	HOH	187	31.190	15.323	75.128	1.00	20.03	O
	HETATM 7466	O	HOH	188	14.972	-3.491	93.351	1.00	14.63	O
	HETATM 7467	O	HOH	189	33.643	-26.102	88.928	1.00	13.28	O
	HETATM 7468	O	HOH	190	14.157	-3.832	83.653	1.00	15.51	O
	HETATM 7469	O	HOH	191	16.075	2.677	84.119	1.00	13.77	O
	HETATM 7470	O	HOH	192	5.961	59.756	86.639	1.00	15.45	O
	HETATM 7471	O	HOH	193	53.593	7.432	73.872	1.00	9.46	O
	HETATM 7472	O	HOH	194	16.552	28.787	80.605	1.00	20.58	O
	HETATM 7473	O	HOH	195	-22.154	61.730	66.879	1.00	19.00	O
	HETATM 7474	O	HOH	196	65.211	23.556	50.589	1.00	12.65	O
	HETATM 7475	O	HOH	197	20.812	-10.237	80.086	1.00	15.99	O
	HETATM 7476	O	HOH	198	12.680	-22.809	92.537	1.00	20.01	O
	HETATM 7477	O	HOH	199	4.860	39.319	100.878	1.00	17.08	O
	HETATM 7478	O	HOH	200	14.643	-8.475	94.915	1.00	16.72	O
	HETATM 7479	O	HOH	201	37.171	-16.695	56.371	1.00	25.94	O
	HETATM 7480	O	HOH	202	3.554	22.859	104.659	1.00	23.27	O
	HETATM 7481	O	HOH	203	13.921	-6.176	85.398	1.00	17.14	O
	HETATM 7482	O	HOH	204	-9.333	36.554	63.643	1.00	13.99	O
	HETATM 7483	O	HOH	205	41.956	-38.297	93.320	1.00	14.96	O
	HETATM 7484	O	HOH	206	12.202	55.926	84.289	1.00	28.63	O
	HETATM 7485	O	HOH	207	32.415	-13.038	57.015	1.00	13.94	O
	HETATM 7486	O	HOH	208	23.428	26.174	70.332	1.00	20.13	O
	HETATM 7487	O	HOH	209	39.691	-2.493	81.540	1.00	12.68	O
	HETATM 7488	O	HOH	210	45.745	6.122	86.144	1.00	15.47	O

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FIG. 53-114	HETATM 7490	O	HOH	212	4.232	41.785	93.744	1.00	11.14	O
	HETATM 7491	O	HOH	213	-26.371	48.653	83.800	1.00	22.33	O
	HETATM 7492	O	HOH	214	35.669	-23.875	104.159	1.00	17.37	O
	HETATM 7493	O	HOH	215	-4.831	41.986	98.947	1.00	15.95	O
	HETATM 7494	O	HOH	216	64.565	-18.038	83.429	1.00	17.54	O
	HETATM 7495	O	HOH	217	11.574	-6.057	93.845	1.00	13.27	O
	HETATM 7496	O	HOH	218	16.307	-18.239	94.494	1.00	19.10	O
	HETATM 7497	O	HOH	219	11.937	69.635	73.406	1.00	19.30	O
	HETATM 7498	O	HOH	220	26.169	-28.822	96.515	1.00	19.46	O
	HETATM 7499	O	HOH	221	67.272	34.853	56.556	1.00	21.78	O
	HETATM 7500	O	HOH	222	-18.977	59.720	77.820	1.00	22.92	O
	HETATM 7501	O	HOH	223	15.918	20.946	99.582	1.00	16.46	O
	HETATM 7502	O	HOH	224	-0.774	60.722	61.425	1.00	13.35	O
	HETATM 7503	O	HOH	225	43.500	-21.837	105.724	1.00	24.80	O
	HETATM 7504	O	HOH	226	-19.597	48.328	89.458	1.00	11.73	O
	HETATM 7505	O	HOH	227	4.976	31.168	72.941	1.00	15.48	O
	HETATM 7506	O	HOH	228	20.015	10.958	62.951	1.00	18.60	O
	HETATM 7507	O	HOH	229	-1.877	27.929	79.869	1.00	11.60	O
	HETATM 7508	O	HOH	230	50.008	-13.926	99.678	1.00	18.48	O
	HETATM 7509	O	HOH	231	53.017	-6.427	76.116	1.00	13.73	O
	HETATM 7510	O	HOH	232	49.120	19.715	51.618	1.00	14.06	O
	HETATM 7511	O	HOH	233	71.110	19.870	50.750	1.00	18.75	O
	HETATM 7512	O	HOH	234	40.374	-37.587	74.192	1.00	31.35	O
	HETATM 7513	O	HOH	235	42.478	-21.001	69.295	1.00	12.38	O
	HETATM 7514	O	HOH	236	7.753	59.653	60.902	1.00	17.67	O
	HETATM 7515	O	HOH	237	21.916	-47.992	76.997	1.00	24.89	O
	HETATM 7516	O	HOH	238	-18.941	54.736	85.871	1.00	20.65	O
	HETATM 7517	O	HOH	239	38.415	-43.269	84.655	1.00	25.51	O
	HETATM 7518	O	HOH	240	-18.492	48.187	61.040	1.00	24.74	O
	HETATM 7519	O	HOH	241	38.277	-50.092	75.188	1.00	19.53	O
	HETATM 7520	O	HOH	242	68.758	16.494	47.667	1.00	18.47	O
	HETATM 7521	O	HOH	243	24.340	-32.949	92.430	1.00	22.79	O
	HETATM 7522	O	HOH	244	6.446	31.879	48.021	1.00	24.85	O
	HETATM 7523	O	HOH	245	28.709	11.531	68.166	1.00	16.31	O
	HETATM 7524	O	HOH	246	31.753	-18.347	108.363	1.00	16.37	O
	HETATM 7525	O	HOH	247	17.759	-8.734	71.761	1.00	26.28	O
	HETATM 7526	O	HOH	248	-25.338	48.165	75.161	1.00	15.71	O
	HETATM 7527	O	HOH	249	67.204	3.621	65.113	1.00	20.08	O
	HETATM 7528	O	HOH	250	3.091	29.574	81.292	1.00	23.58	O
	HETATM 7529	O	HOH	251	29.230	-25.705	89.928	1.00	18.11	O
	HETATM 7530	O	HOH	252	20.116	-6.764	65.412	1.00	16.66	O
	HETATM 7531	O	HOH	253	29.673	-12.800	109.481	1.00	20.49	O
	HETATM 7532	O	HOH	254	25.768	10.314	72.068	1.00	13.03	O
	HETATM 7533	O	HOH	255	61.202	29.626	44.098	1.00	21.43	O
	HETATM 7534	O	HOH	256	2.263	24.087	69.363	1.00	14.58	O
	HETATM 7535	O	HOH	257	-3.037	70.229	83.110	1.00	21.27	O
	HETATM 7536	O	HOH	258	72.666	33.964	61.263	1.00	36.04	O
	HETATM 7537	O	HOH	259	4.432	16.319	101.738	1.00	16.96	O
	HETATM 7538	O	HOH	260	-13.423	48.880	72.973	1.00	24.01	O
	HETATM 7539	O	HOH	261	-4.663	58.301	66.514	1.00	15.31	O
	HETATM 7540	O	HOH	262	40.987	-35.386	93.294	1.00	22.01	O
	HETATM 7541	O	HOH	263	-11.233	62.808	76.653	1.00	24.18	O
	HETATM 7542	O	HOH	264	24.821	0.548	61.582	1.00	21.73	O
	HETATM 7543	O	HOH	265	24.965	29.544	79.722	1.00	22.80	O
	HETATM 7544	O	HOH	266	-5.380	3.025	75.813	1.00	22.22	O
	HETATM 7545	O	HOH	267	24.742	-24.647	89.587	1.00	20.25	O
	HETATM 7546	O	HOH	268	65.140	7.222	49.806	1.00	15.66	O
	HETATM 7547	O	HOH	269	41.346	-10.499	81.998	1.00	18.92	O
	HETATM 7548	O	HOH	270	66.840	21.038	63.543	1.00	13.26	O
	HETATM 7549	O	HOH	271	51.301	-14.931	69.495	1.00	22.63	O
	HETATM 7550	O	HOH	272	29.219	-0.500	64.123	1.00	19.73	O
	HETATM 7551	O	HOH	273	20.241	6.270	63.246	1.00	13.54	O
	HETATM 7552	O	HOH	274	24.373	-49.590	68.733	1.00	17.26	O
	HETATM 7553	O	HOH	275	-3.304	48.988	55.440	1.00	31.16	O
	HETATM 7554	O	HOH	276	20.108	7.029	66.151	1.00	16.95	O
	HETATM 7555	O	HOH	277	7.782	-18.762	93.633	1.00	26.41	O
	HETATM 7556	O	HOH	278	27.949	-0.521	45.474	1.00	22.32	O
	HETATM 7557	O	HOH	279	31.631	6.490	78.024	1.00	21.67	O
	HETATM 7558	O	HOH	280	23.318	29.759	69.062	1.00	22.20	O
	HETATM 7559	O	HOH	281	-6.248	20.741	81.137	1.00	24.62	O

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FIG. 53-115	HETATM 7561	O	HOH	283	52.122	-23.691	79.136	1.00	23.09	O
	HETATM 7562	O	HOH	284	70.779	32.618	51.713	1.00	17.19	O
	HETATM 7563	O	HOH	285	63.452	0.172	52.716	1.00	33.32	O
	HETATM 7564	O	HOH	286	22.958	-47.681	67.413	1.00	22.89	O
	HETATM 7565	O	HOH	287	23.890	32.593	72.960	1.00	22.24	O
	HETATM 7566	O	HOH	288	20.986	30.840	66.080	1.00	21.84	O
	HETATM 7567	O	HOH	289	-9.603	65.551	84.452	1.00	25.25	O
	HETATM 7568	O	HOH	290	28.073	-23.477	89.005	1.00	18.93	O
	HETATM 7569	O	HOH	291	55.835	10.701	63.810	1.00	20.35	O
	HETATM 7570	O	HOH	292	9.046	17.920	56.027	1.00	15.93	O
	HETATM 7571	O	HOH	293	28.350	-18.254	64.363	1.00	15.02	O
	HETATM 7572	O	HOH	294	-0.201	3.801	81.142	1.00	16.11	O
	HETATM 7573	O	HOH	295	46.141	-21.508	105.098	1.00	16.42	O
	HETATM 7574	O	HOH	296	13.399	-22.499	76.433	1.00	25.53	O
	HETATM 7575	O	HOH	297	24.981	-30.380	92.166	1.00	33.02	O
	HETATM 7576	O	HOH	298	13.771	56.074	62.370	1.00	19.18	O
	HETATM 7577	O	HOH	299	-8.893	35.838	86.208	1.00	20.61	O
	HETATM 7578	O	HOH	300	-22.126	64.290	67.305	1.00	19.81	O
	HETATM 7579	O	HOH	301	33.698	-14.983	108.516	1.00	14.40	O
	HETATM 7580	O	HOH	302	42.101	-11.945	58.376	1.00	20.92	O
	HETATM 7581	O	HOH	303	-18.526	61.045	73.900	1.00	32.62	O
	HETATM 7582	O	HOH	304	3.513	24.995	102.792	1.00	23.31	O
	HETATM 7583	O	HOH	305	20.343	18.184	93.670	1.00	17.08	O
	HETATM 7584	O	HOH	306	5.882	55.992	87.891	1.00	30.47	O
	HETATM 7585	O	HOH	307	-9.244	36.503	67.888	1.00	28.48	O
	HETATM 7586	O	HOH	308	-23.036	58.479	59.552	1.00	22.63	O
	HETATM 7587	O	HOH	309	-22.227	45.809	59.422	1.00	21.33	O
	HETATM 7588	O	HOH	310	53.262	10.903	71.166	1.00	17.46	O
	HETATM 7589	O	HOH	311	52.602	26.636	60.251	1.00	25.23	O
	HETATM 7590	O	HOH	312	-9.994	55.398	87.998	1.00	17.49	O
	HETATM 7591	O	HOH	313	-1.994	61.292	66.107	1.00	21.25	O
	HETATM 7592	O	HOH	314	50.016	-11.293	93.731	1.00	24.97	O
	HETATM 7593	O	HOH	315	15.116	16.011	100.168	1.00	15.56	O
	HETATM 7594	O	HOH	316	-6.826	24.369	98.991	1.00	22.05	O
	HETATM 7595	O	HOH	317	2.708	42.709	80.252	1.00	17.54	O
	HETATM 7596	O	HOH	318	1.253	20.189	100.045	1.00	15.04	O
	HETATM 7597	O	HOH	319	5.356	34.912	77.758	1.00	13.93	O
	HETATM 7598	O	HOH	320	28.400	23.106	67.434	1.00	26.44	O
	HETATM 7599	O	HOH	321	9.493	-19.687	95.975	1.00	31.85	O
	HETATM 7600	O	HOH	322	54.155	24.844	62.487	1.00	16.62	O
	HETATM 7601	O	HOH	323	46.411	-19.574	59.883	1.00	31.91	O
	HETATM 7602	O	HOH	324	-9.761	37.077	89.314	1.00	28.06	O
	HETATM 7603	O	HOH	325	17.686	-11.211	73.805	1.00	18.94	O
	HETATM 7604	O	HOH	326	1.967	43.860	93.220	1.00	18.25	O
	HETATM 7605	O	HOH	327	6.187	59.026	91.814	1.00	28.67	O
	HETATM 7606	O	HOH	328	37.107	-14.358	54.717	1.00	22.03	O
	HETATM 7607	O	HOH	329	38.785	-11.357	84.088	1.00	16.84	O
	HETATM 7608	O	HOH	330	-16.066	60.369	76.960	1.00	36.78	O
	HETATM 7609	O	HOH	331	-5.054	1.253	78.433	1.00	25.45	O
	HETATM 7610	O	HOH	332	11.331	-12.981	75.925	1.00	14.82	O
	HETATM 7611	O	HOH	333	32.919	-41.920	95.418	1.00	27.83	O
	HETATM 7612	O	HOH	334	-14.341	51.888	93.906	1.00	24.92	O
	HETATM 7613	O	HOH	335	53.967	-0.127	74.878	1.00	28.14	O
	HETATM 7614	O	HOH	336	12.881	-19.058	86.018	1.00	23.40	O
	HETATM 7615	O	HOH	337	5.705	51.167	93.636	1.00	19.15	O
	HETATM 7616	O	HOH	338	42.319	-33.425	91.495	1.00	24.82	O
	HETATM 7617	O	HOH	339	2.306	38.419	86.466	1.00	19.39	O
	HETATM 7618	O	HOH	340	43.350	-13.777	74.954	1.00	21.98	O
	HETATM 7619	O	HOH	341	33.960	-34.534	91.429	1.00	29.34	O
	HETATM 7620	O	HOH	342	4.202	62.085	62.525	1.00	26.90	O
	HETATM 7621	O	HOH	343	30.962	-34.415	78.307	1.00	19.88	O
	HETATM 7622	O	HOH	344	35.773	-42.848	100.309	1.00	30.39	O
	HETATM 7623	O	HOH	345	12.021	-37.942	70.940	1.00	20.13	O
	HETATM 7624	O	HOH	346	-1.357	49.449	58.279	1.00	25.11	O
	HETATM 7625	O	HOH	347	65.788	2.612	67.270	1.00	26.50	O
	HETATM 7626	O	HOH	348	62.163	0.051	71.262	1.00	14.33	O
	HETATM 7627	O	HOH	349	3.350	45.790	78.716	1.00	19.58	O
	HETATM 7628	O	HOH	350	45.104	-33.566	100.903	1.00	25.20	O
	HETATM 7629	O	HOH	351	43.597	-0.623	84.186	1.00	28.63	O
	HETATM 7630	O	HOH	352	4.596	12.242	87.087	1.00	25.56	O

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FIG. 53-116

HETATM 7632	O	HOH	354	1.875	10.993	64.255	1.00	38.92	O
HETATM 7633	O	HOH	355	14.789	30.075	58.623	1.00	21.49	O
HETATM 7634	O	HOH	356	41.516	-25.204	62.351	1.00	22.09	O
HETATM 7635	O	HOH	357	32.943	-23.386	104.220	1.00	27.01	O
HETATM 7636	O	HOH	358	-10.674	42.191	63.227	1.00	19.76	O
HETATM 7637	O	HOH	359	-13.052	65.840	75.218	1.00	29.44	O
HETATM 7638	O	HOH	360	37.573	-17.256	81.764	1.00	27.76	O
HETATM 7639	O	HOH	361	20.895	9.352	68.130	1.00	16.95	O
HETATM 7640	O	HOH	362	-27.567	46.850	73.499	1.00	27.75	O
HETATM 7641	O	HOH	363	8.363	27.062	51.462	1.00	23.49	O
HETATM 7642	O	HOH	364	20.807	-20.790	92.215	1.00	13.77	O
HETATM 7643	O	HOH	365	38.677	-18.189	74.814	1.00	28.95	O
HETATM 7644	O	HOH	366	-2.447	43.907	70.580	1.00	29.93	O
HETATM 7645	O	HOH	367	64.618	-6.837	66.273	1.00	29.07	O
HETATM 7646	O	HOH	368	-5.882	37.844	71.080	1.00	16.09	O
HETATM 7647	O	HOH	369	11.154	36.109	99.944	1.00	28.58	O
HETATM 7648	O	HOH	370	-5.542	16.069	77.059	1.00	25.73	O
HETATM 7649	O	HOH	371	31.111	-16.478	52.927	1.00	31.54	O
HETATM 7650	O	HOH	372	5.976	50.145	55.972	1.00	20.23	O
HETATM 7651	O	HOH	373	22.475	-11.962	59.589	1.00	25.23	O
HETATM 7652	O	HOH	374	-12.598	60.928	80.629	1.00	31.48	O
HETATM 7653	O	HOH	375	39.980	-5.340	88.804	1.00	25.19	O
HETATM 7654	O	HOH	376	-2.191	22.122	77.573	1.00	19.70	O
HETATM 7655	O	HOH	377	-1.570	23.321	89.728	1.00	27.93	O
HETATM 7656	O	HOH	378	33.278	2.409	86.604	1.00	20.38	O
HETATM 7657	O	HOH	379	39.069	-36.284	69.975	1.00	35.94	O
HETATM 7658	O	HOH	380	37.465	-16.311	88.358	1.00	25.21	O
HETATM 7659	O	HOH	381	-16.777	66.073	65.338	1.00	23.04	O
HETATM 7660	O	HOH	382	64.525	-20.940	83.663	1.00	32.87	O
HETATM 7661	O	HOH	383	20.902	-16.651	86.838	1.00	21.83	O
HETATM 7662	O	HOH	384	17.379	15.560	98.403	1.00	36.64	O
HETATM 7663	O	HOH	385	52.346	-11.927	82.994	1.00	24.35	O
HETATM 7664	O	HOH	386	33.051	-14.312	69.234	1.00	23.31	O
HETATM 7665	O	HOH	387	18.244	-50.461	70.951	1.00	32.07	O
HETATM 7666	O	HOH	388	4.393	13.312	75.485	1.00	27.15	O
HETATM 7667	O	HOH	389	67.585	44.217	58.028	1.00	44.96	O
HETATM 7668	O	HOH	390	4.131	14.065	99.710	1.00	26.76	O
HETATM 7669	O	HOH	391	11.175	-0.969	70.399	1.00	26.13	O
HETATM 7670	O	HOH	392	51.116	-18.029	102.066	1.00	23.76	O
HETATM 7671	O	HOH	393	27.092	-7.580	108.056	1.00	18.96	O
HETATM 7672	O	HOH	394	-0.076	36.263	69.351	1.00	28.76	O
HETATM 7673	O	HOH	395	18.133	0.192	74.686	1.00	26.61	O
HETATM 7674	O	HOH	396	43.049	2.569	79.498	1.00	31.94	O
HETATM 7675	O	HOH	397	-23.286	56.992	79.188	1.00	29.11	O
HETATM 7676	O	HOH	398	-7.488	11.902	76.612	1.00	26.52	O
HETATM 7677	O	HOH	399	-13.380	61.310	72.384	1.00	31.14	O
HETATM 7678	O	HOH	400	27.123	-46.681	87.721	1.00	30.44	O
HETATM 7679	O	HOH	401	29.433	-31.173	89.189	1.00	25.67	O
HETATM 7680	O	HOH	402	52.760	-20.241	79.508	1.00	13.02	O
HETATM 7681	O	HOH	403	-1.394	34.237	85.422	1.00	22.50	O
HETATM 7682	O	HOH	404	23.304	-20.804	99.890	1.00	21.06	O
HETATM 7683	O	HOH	405	10.950	27.172	54.652	1.00	26.13	O
HETATM 7684	O	HOH	406	17.093	-18.459	105.982	1.00	38.33	O
HETATM 7685	O	HOH	407	29.611	-46.659	90.122	1.00	22.95	O
HETATM 7686	O	HOH	408	10.218	70.152	76.785	1.00	48.49	O
HETATM 7687	O	HOH	409	60.036	-4.064	49.508	1.00	35.97	O
HETATM 7688	O	HOH	410	51.542	-26.357	92.153	1.00	37.00	O
HETATM 7689	O	HOH	411	43.954	-25.924	102.957	1.00	25.36	O
HETATM 7690	O	HOH	412	8.761	46.091	74.278	1.00	21.32	O
HETATM 7691	O	HOH	413	25.286	-20.091	69.480	1.00	15.27	O
HETATM 7692	O	HOH	414	65.539	40.531	49.494	1.00	31.85	O
HETATM 7693	O	HOH	415	44.413	-32.734	84.479	1.00	28.75	O
HETATM 7694	O	HOH	416	-5.043	18.491	79.930	1.00	30.44	O
HETATM 7695	O	HOH	417	-3.086	39.625	75.814	1.00	29.90	O
HETATM 7696	O	HOH	418	58.905	-24.381	86.911	1.00	35.04	O
HETATM 7697	O	HOH	419	44.458	-29.330	96.836	1.00	29.99	O
HETATM 7698	O	HOH	420	-19.898	62.569	69.832	1.00	34.66	O
HETATM 7699	O	HOH	421	21.778	-33.633	73.728	1.00	29.63	O
HETATM 7700	O	HOH	422	28.583	-8.540	66.452	1.00	42.51	O
HETATM 7701	O	HOH	423	46.541	9.226	72.812	1.00	42.38	O

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FIG. 53-117

HETATM 7703	O	HOH	425	38.290	-25.478	102.465	1.00	30.41	O
HETATM 7704	O	HOH	426	19.472	-12.973	106.738	1.00	26.85	O
HETATM 7705	O	HOH	427	62.854	11.594	46.547	1.00	26.89	O
HETATM 7706	O	HOH	428	31.588	-16.806	71.522	1.00	24.18	O
HETATM 7707	O	HOH	429	13.954	13.665	81.796	1.00	24.37	O
HETATM 7708	O	HOH	430	2.011	5.974	84.071	1.00	28.86	O
HETATM 7709	O	HOH	431	7.560	21.926	104.239	1.00	34.95	O
HETATM 7710	O	HOH	432	14.098	-7.313	91.358	1.00	22.24	O
HETATM 7711	O	HOH	433	32.623	-2.548	91.064	1.00	24.03	O
HETATM 7712	O	HOH	434	4.401	54.311	60.091	1.00	22.83	O
HETATM 7713	O	HOH	435	4.015	35.675	104.766	1.00	19.87	O
HETATM 7714	O	HOH	436	-17.908	53.196	92.502	1.00	38.80	O
HETATM 7715	O	HOH	437	27.675	-50.214	83.317	1.00	28.60	O
HETATM 7716	O	HOH	438	-11.291	59.604	78.311	1.00	16.91	O
HETATM 7717	O	HOH	439	31.453	1.868	91.380	1.00	28.49	O
HETATM 7718	O	HOH	440	-11.594	70.398	81.234	1.00	31.72	O
HETATM 7719	O	HOH	441	46.134	-11.872	61.301	1.00	21.50	O
HETATM 7720	O	HOH	442	11.900	35.238	64.506	1.00	23.66	O
HETATM 7721	O	HOH	443	4.846	10.765	96.924	1.00	34.00	O
HETATM 7722	O	HOH	444	-18.730	59.840	58.173	1.00	43.07	O
HETATM 7723	O	HOH	445	57.404	-16.056	75.983	1.00	42.76	O
HETATM 7724	O	HOH	446	29.809	-16.290	111.959	1.00	48.83	O
HETATM 7725	O	HOH	447	32.033	-44.011	72.701	1.00	24.09	O
HETATM 7726	O	HOH	448	20.875	-24.975	70.063	1.00	48.89	O
HETATM 7727	O	HOH	449	-19.969	46.503	77.606	1.00	25.87	O
HETATM 7728	O	HOH	450	-21.566	54.606	85.472	1.00	40.92	O
HETATM 7729	O	HOH	451	31.102	-32.885	98.369	1.00	11.96	O
HETATM 7730	O	HOH	452	-8.189	9.765	80.662	1.00	35.27	O
HETATM 7731	O	HOH	453	31.340	-19.222	51.487	1.00	24.37	O
HETATM 7732	O	HOH	454	29.058	-28.472	89.087	1.00	26.15	O
HETATM 7733	O	HOH	455	-2.419	36.836	105.573	1.00	27.97	O
HETATM 7734	O	HOH	456	21.812	-9.184	104.095	1.00	27.13	O
HETATM 7735	O	HOH	457	49.451	-20.677	84.809	1.00	41.47	O
HETATM 7736	O	HOH	458	0.747	30.885	63.795	1.00	31.04	O
HETATM 7737	O	HOH	459	-26.174	50.602	73.929	1.00	53.06	O
HETATM 7738	O	HOH	460	8.337	72.878	75.753	1.00	38.38	O
HETATM 7739	O	HOH	461	23.508	-2.410	57.597	1.00	46.06	O
HETATM 7740	O	HOH	462	37.169	-45.172	99.612	1.00	37.17	O
HETATM 7741	O	HOH	463	22.696	-4.544	56.151	1.00	47.00	O
HETATM 7742	O	HOH	464	21.082	-23.510	106.197	1.00	22.09	O
HETATM 7743	O	HOH	465	-3.315	21.210	61.358	1.00	27.90	O
HETATM 7744	O	HOH	466	25.279	-14.132	96.196	1.00	28.85	O
HETATM 7745	O	HOH	467	63.921	40.060	58.906	1.00	35.83	O
HETATM 7746	O	HOH	468	14.094	-6.423	88.307	1.00	44.69	O
HETATM 7747	O	HOH	469	25.519	1.763	92.408	1.00	24.38	O
HETATM 7748	O	HOH	470	50.197	11.830	54.707	1.00	28.25	O
HETATM 7749	O	HOH	471	21.550	31.794	76.291	1.00	21.43	O
HETATM 7750	O	HOH	472	26.886	-15.693	73.749	1.00	41.24	O
HETATM 7751	O	HOH	473	14.177	31.775	80.787	1.00	46.37	O
HETATM 7752	O	HOH	474	-13.585	38.871	87.985	1.00	32.09	O
HETATM 7753	O	HOH	475	41.661	-21.201	71.774	1.00	34.90	O
HETATM 7754	O	HOH	476	48.196	-33.291	70.217	1.00	37.35	O
HETATM 7755	O	HOH	477	0.248	5.883	79.177	1.00	23.06	O
HETATM 7756	O	HOH	478	-20.978	57.784	74.179	1.00	45.09	O
HETATM 7757	O	HOH	479	15.338	14.734	57.576	1.00	27.62	O
HETATM 7758	O	HOH	480	39.859	-43.440	87.980	1.00	30.78	O
HETATM 7759	O	HOH	481	5.332	35.152	64.988	1.00	33.57	O
HETATM 7760	O	HOH	482	32.546	-7.422	108.285	1.00	41.57	O
HETATM 7761	O	HOH	483	20.706	43.978	65.616	1.00	37.68	O
HETATM 7762	O	HOH	484	61.667	39.679	46.403	1.00	37.33	O
HETATM 7763	O	HOH	485	56.153	6.917	74.246	1.00	22.50	O
HETATM 7764	O	HOH	486	7.035	69.370	79.949	1.00	25.17	O
HETATM 7765	O	HOH	487	57.622	33.652	55.881	1.00	33.26	O
HETATM 7766	O	HOH	488	18.571	3.099	54.965	1.00	33.08	O
HETATM 7767	O	HOH	489	0.917	22.142	67.869	1.00	27.76	O
HETATM 7768	O	HOH	490	-10.181	67.927	72.593	1.00	37.33	O
HETATM 7769	O	HOH	491	-1.369	19.165	63.747	1.00	42.82	O
HETATM 7770	O	HOH	492	-2.905	16.592	80.047	1.00	27.79	O
HETATM 7771	O	HOH	493	71.624	17.692	61.442	1.00	30.28	O
HETATM 7772	O	HOH	494	10.080	44.711	55.632	1.00	34.86	O

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FIG. 53-118

HETATM 7774	O	HOH	496	56.970	20.418	62.613	1.00	43.51	O
HETATM 7775	O	HOH	497	7.317	61.022	83.606	1.00	30.90	O
HETATM 7776	O	HOH	498	-20.765	57.011	50.630	1.00	30.28	O
HETATM 7777	O	HOH	499	5.680	-5.938	83.013	1.00	33.85	O
HETATM 7778	O	HOH	500	10.160	33.195	64.242	1.00	33.78	O
HETATM 7779	O	HOH	501	-3.876	47.464	68.947	1.00	35.45	O
HETATM 7780	O	HOH	502	25.895	-25.113	107.060	1.00	31.04	O
HETATM 7781	O	HOH	503	25.954	-25.486	96.235	1.00	41.89	O
HETATM 7782	O	HOH	504	11.628	-8.334	83.763	1.00	37.43	O
HETATM 7783	O	HOH	505	20.353	-25.228	99.439	1.00	28.33	O
HETATM 7784	O	HOH	506	74.272	26.082	49.678	1.00	23.93	O
HETATM 7785	O	HOH	507	21.208	-4.593	103.849	1.00	35.84	O
HETATM 7786	O	HOH	508	-11.137	31.147	89.386	1.00	37.60	O
HETATM 7787	O	HOH	509	2.586	5.500	73.452	1.00	22.80	O
HETATM 7788	O	HOH	510	65.236	-3.380	56.556	1.00	40.70	O
HETATM 7789	O	HOH	511	41.003	-32.111	78.380	1.00	43.60	O
HETATM 7790	O	HOH	512	36.216	-35.399	72.031	1.00	27.60	O
HETATM 7791	O	HOH	513	19.195	29.924	79.296	1.00	54.45	O
HETATM 7792	O	HOH	514	33.620	-39.417	97.385	1.00	19.90	O
HETATM 7793	O	HOH	515	42.416	-2.969	83.920	1.00	35.14	O
HETATM 7794	O	HOH	516	17.949	-13.685	90.670	1.00	40.03	O
HETATM 7795	O	HOH	517	3.575	51.449	55.759	1.00	26.16	O
HETATM 7796	O	HOH	518	11.256	2.878	84.105	1.00	23.64	O
HETATM 7797	O	HOH	519	-12.990	55.942	83.392	1.00	29.31	O
HETATM 7798	O	HOH	520	23.910	-7.458	59.473	1.00	49.79	O
HETATM 7799	O	HOH	521	-0.082	9.238	75.111	1.00	30.80	O
HETATM 7800	O	HOH	522	-11.514	65.215	81.280	1.00	40.25	O
HETATM 7801	O	HOH	523	1.302	12.024	74.914	1.00	22.96	O
HETATM 7802	O	HOH	524	-12.681	60.508	63.319	1.00	35.93	O
HETATM 7803	O	HOH	525	26.972	-49.547	86.691	1.00	28.47	O
HETATM 7804	O	HOH	526	27.537	25.048	86.077	1.00	34.16	O
HETATM 7805	O	HOH	527	6.797	56.961	61.831	1.00	42.31	O
HETATM 7806	O	HOH	528	42.484	-2.653	58.047	1.00	40.72	O
HETATM 7807	O	HOH	529	-18.325	52.964	53.615	1.00	39.32	O
HETATM 7808	O	HOH	530	31.179	-21.542	61.949	1.00	33.36	O
HETATM 7809	O	HOH	531	11.810	67.897	76.687	1.00	31.68	O
HETATM 7810	O	HOH	532	7.417	5.985	71.567	1.00	32.02	O
HETATM 7811	O	HOH	533	-21.963	59.779	80.267	1.00	19.20	O
HETATM 7812	O	HOH	534	25.891	3.913	54.668	1.00	39.82	O
HETATM 7813	O	HOH	535	11.470	61.996	73.117	1.00	38.96	O
HETATM 7814	O	HOH	536	32.905	-1.708	70.903	1.00	33.03	O
HETATM 7815	O	HOH	537	44.005	-23.045	60.071	1.00	40.10	O
HETATM 7816	O	HOH	538	-10.255	28.829	87.634	1.00	36.10	O
HETATM 7817	O	HOH	539	16.712	-10.311	97.916	1.00	33.61	O
HETATM 7818	O	HOH	540	41.339	1.249	74.690	1.00	28.48	O
HETATM 7819	O	HOH	541	-1.348	71.272	76.255	1.00	25.11	O
HETATM 7820	O	HOH	542	34.260	17.004	67.448	1.00	38.74	O
HETATM 7821	O	HOH	543	11.605	5.120	70.043	1.00	38.08	O
HETATM 7822	O	HOH	544	52.550	-9.796	53.931	1.00	35.58	O
HETATM 7823	O	HOH	545	14.247	54.880	59.924	1.00	32.50	O
HETATM 7824	O	HOH	546	-2.549	46.429	71.418	1.00	32.37	O
HETATM 7825	O	HOH	547	12.782	-40.884	84.382	1.00	24.04	O
HETATM 7826	O	HOH	548	-25.600	44.661	65.942	1.00	27.28	O
HETATM 7827	O	HOH	549	27.739	-35.104	72.246	1.00	41.35	O
HETATM 7828	O	HOH	550	73.990	31.829	50.606	1.00	36.92	O
HETATM 7829	O	HOH	551	12.894	-10.737	95.923	1.00	36.10	O
HETATM 7830	O	HOH	552	46.236	-9.151	59.517	1.00	38.03	O
HETATM 7831	O	HOH	553	14.123	42.425	67.129	1.00	52.00	O
HETATM 7832	O	HOH	554	-23.813	46.436	79.979	1.00	37.72	O
HETATM 7833	O	HOH	555	-26.297	58.232	78.735	1.00	29.43	O
HETATM 7834	O	HOH	556	35.090	-43.947	90.740	1.00	37.16	O
HETATM 7835	O	HOH	557	66.933	8.617	46.645	1.00	22.50	O
HETATM 7836	O	HOH	558	33.659	-6.348	111.290	1.00	33.71	O
HETATM 7837	O	HOH	559	22.491	-13.967	105.700	1.00	33.38	O
HETATM 7838	O	HOH	560	12.516	-5.293	101.139	1.00	38.89	O
HETATM 7839	O	HOH	561	10.978	32.220	73.143	1.00	39.37	O
HETATM 7840	O	HOH	562	55.531	-10.263	54.745	1.00	41.91	O
HETATM 7841	O	HOH	563	-8.024	12.880	90.645	1.00	33.15	O
HETATM 7842	O	HOH	564	14.873	18.651	98.780	1.00	32.24	O
HETATM 7843	O	HOH	565	41.000	-14.756	57.520	1.00	34.60	O

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FIG. 53-119

HETATM 7845	O	HOH	567	36.171	-1.816	61.767	1.00	31.43	O
HETATM 7846	O	HOH	568	44.474	-26.007	60.823	1.00	34.19	O
HETATM 7847	O	HOH	569	20.938	-46.385	85.402	1.00	29.47	O
HETATM 7848	O	HOH	570	52.948	8.143	71.171	1.00	34.33	O
HETATM 7849	O	HOH	571	51.129	-7.179	82.571	1.00	47.80	O
HETATM 7850	O	HOH	572	68.198	2.685	52.665	1.00	23.57	O
HETATM 7851	O	HOH	573	12.116	71.650	75.451	1.00	46.93	O
HETATM 7852	O	HOH	574	62.213	37.792	48.687	1.00	53.82	O
HETATM 7853	O	HOH	575	20.495	10.177	90.640	1.00	39.16	O
HETATM 7854	O	HOH	576	30.400	-48.938	83.842	1.00	35.90	O
HETATM 7855	O	HOH	577	13.579	9.779	62.019	1.00	44.35	O
HETATM 7856	O	HOH	578	10.453	26.949	106.358	1.00	40.82	O
HETATM 7857	O	HOH	579	60.381	11.598	69.404	1.00	34.68	O
HETATM 7858	O	HOH	580	25.629	2.637	73.266	1.00	36.83	O
HETATM 7859	O	HOH	581	32.166	-30.120	78.054	1.00	37.93	O
HETATM 7860	O	HOH	582	-22.014	44.722	62.268	1.00	30.72	O
HETATM 7861	O	HOH	583	11.801	31.240	55.851	1.00	44.26	O
HETATM 7862	O	HOH	584	18.441	-32.822	78.003	1.00	44.37	O
HETATM 7863	O	HOH	585	30.789	22.569	66.579	1.00	46.89	O
HETATM 7864	O	HOH	586	37.285	-23.655	106.529	1.00	30.28	O
HETATM 7865	O	HOH	587	51.534	10.981	63.481	1.00	32.89	O
HETATM 7866	O	HOH	588	49.912	3.080	78.435	1.00	47.56	O
HETATM 7867	O	HOH	589	34.134	-20.660	68.829	1.00	36.65	O
HETATM 7868	O	HOH	590	37.754	-14.502	81.017	1.00	37.24	O
HETATM 7869	O	HOH	591	36.512	-49.054	82.287	1.00	45.12	O
HETATM 7870	O	HOH	592	-5.195	45.154	64.492	1.00	33.46	O
HETATM 7871	O	HOH	593	23.758	-22.142	68.735	1.00	46.87	O
HETATM 7872	O	HOH	594	11.629	38.685	97.627	1.00	33.19	O
HETATM 7873	O	HOH	595	21.263	2.941	69.561	1.00	39.33	O
HETATM 7874	O	HOH	596	73.271	25.458	53.024	1.00	25.93	O
HETATM 7875	O	HOH	597	45.849	-7.205	101.568	1.00	36.34	O
HETATM 7876	O	HOH	598	44.216	-10.630	108.940	1.00	43.94	O
HETATM 7877	O	HOH	599	59.076	-22.331	92.759	1.00	47.77	O
HETATM 7878	O	HOH	600	54.559	-30.657	83.945	1.00	59.82	O
HETATM 7879	O	HOH	601	-1.816	16.701	100.021	1.00	52.67	O
HETATM 7880	O	HOH	602	58.154	31.812	65.596	1.00	52.96	O
HETATM 7881	O	HOH	1000	26.160	-11.235	84.250	0.00	0.00	O
CONNECT 255			254	402					
CONNECT 307			306	339					
CONNECT 339			307	338					
CONNECT 347			345	2302					
CONNECT 402			255	401					
CONNECT 509			508	713					
CONNECT 577			576	656					
CONNECT 628			626	2316					
CONNECT 656			577	655					
CONNECT 713			509	712					
CONNECT 828			826	2330					
CONNECT 932			930	2344					
CONNECT 1035			1033	2358					
CONNECT 1080			1078	2372					
CONNECT 1086			1085	1122					
CONNECT 1122			1086	1121					
CONNECT 1130			1128	2386					
CONNECT 1191			1189	2400					
CONNECT 1496			1495	1926					
CONNECT 1553			1552	1709					
CONNECT 1561			1559	2414					
CONNECT 1610			1608	2428					
CONNECT 1709			1553	1708					
CONNECT 1926			1496	1925					
CONNECT 1946			1944	2442					
CONNECT 2302			347	2303	2313				
CONNECT 2303			2302	2304	2310				
CONNECT 2304			2303	2305	2311				
CONNECT 2305			2304	2306	2312				
CONNECT 2306			2305	2307	2313				
CONNECT 2307			2306	2314					
CONNECT 2308			2309	2310	2315				
CONNECT 2309			2310	2316					



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FIG. 53-120

CONNECT 2311 2304  
CONNECT 2312 2305  
CONNECT 2313 2302 2306  
CONNECT 2314 2307  
CONNECT 2315 2308  
CONNECT 2316 628 2317 2327  
CONNECT 2317 2316 2318 2324  
CONNECT 2318 2317 2319 2325  
CONNECT 2319 2318 2320 2326  
CONNECT 2320 2319 2321 2327  
CONNECT 2321 2320 2328  
CONNECT 2322 2323 2324 2329  
CONNECT 2323 2322  
CONNECT 2324 2317 2322  
CONNECT 2325 2318  
CONNECT 2326 2319  
CONNECT 2327 2316 2320  
CONNECT 2328 2321 2456  
CONNECT 2329 2322  
CONNECT 2330 828 2331 2341  
CONNECT 2331 2330 2332 2338  
CONNECT 2332 2331 2333 2339  
CONNECT 2333 2332 2334 2340  
CONNECT 2334 2333 2335 2341  
CONNECT 2335 2334 2342  
CONNECT 2336 2337 2338 2343  
CONNECT 2337 2336  
CONNECT 2338 2331 2336  
CONNECT 2339 2332  
CONNECT 2340 2333  
CONNECT 2341 2330 2334  
CONNECT 2342 2335  
CONNECT 2343 2336  
CONNECT 2344 932 2345 2355  
CONNECT 2345 2344 2346 2352  
CONNECT 2346 2345 2347 2353  
CONNECT 2347 2346 2348 2354  
CONNECT 2348 2347 2349 2355  
CONNECT 2349 2348 2356  
CONNECT 2350 2351 2352 2357  
CONNECT 2351 2350  
CONNECT 2352 2345 2350  
CONNECT 2353 2346  
CONNECT 2354 2347  
CONNECT 2355 2344 2348  
CONNECT 2356 2349  
CONNECT 2357 2350  
CONNECT 2358 1035 2359 2369  
CONNECT 2359 2358 2360 2366  
CONNECT 2360 2359 2361 2367  
CONNECT 2361 2360 2362 2368  
CONNECT 2362 2361 2363 2369  
CONNECT 2363 2362 2370  
CONNECT 2364 2365 2366 2371  
CONNECT 2365 2364  
CONNECT 2366 2359 2364  
CONNECT 2367 2360  
CONNECT 2368 2361  
CONNECT 2369 2358 2362  
CONNECT 2370 2363  
CONNECT 2371 2364  
CONNECT 2372 1080 2373 2383  
CONNECT 2373 2372 2374 2380  
CONNECT 2374 2373 2375 2381  
CONNECT 2375 2374 2376 2382  
CONNECT 2376 2375 2377 2383  
CONNECT 2377 2376 2384  
CONNECT 2378 2379 2380 2385  
CONNECT 2379 2378  
CONNECT 2380 2379 2378

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FIG. 53-121

CONNECT 2382 2375  
CONNECT 2383 2372 2376  
CONNECT 2384 2377 2466  
CONNECT 2385 2378  
CONNECT 2386 1130 2387 2397  
CONNECT 2387 2386 2388 2394  
CONNECT 2388 2387 2389 2395  
CONNECT 2389 2388 2390 2396  
CONNECT 2390 2389 2391 2397  
CONNECT 2391 2390 2398  
CONNECT 2392 2393 2394 2399  
CONNECT 2393 2392  
CONNECT 2394 2387 2392  
CONNECT 2395 2388  
CONNECT 2396 2389  
CONNECT 2397 2386 2390  
CONNECT 2398 2391  
CONNECT 2399 2392  
CONNECT 2400 1191 2401 2411  
CONNECT 2401 2400 2402 2408  
CONNECT 2402 2401 2403 2409  
CONNECT 2403 2402 2404 2410  
CONNECT 2404 2403 2405 2411  
CONNECT 2405 2404 2412  
CONNECT 2406 2407 2408 2413  
CONNECT 2407 2406  
CONNECT 2408 2401 2406  
CONNECT 2409 2402  
CONNECT 2410 2403  
CONNECT 2411 2400 2404  
CONNECT 2412 2405  
CONNECT 2413 2406  
CONNECT 2414 1561 2415 2425  
CONNECT 2415 2414 2416 2422  
CONNECT 2416 2415 2417 2423  
CONNECT 2417 2416 2418 2424  
CONNECT 2418 2417 2419 2425  
CONNECT 2419 2418 2426  
CONNECT 2420 2421 2422 2427  
CONNECT 2421 2420  
CONNECT 2422 2415 2420  
CONNECT 2423 2416  
CONNECT 2424 2417  
CONNECT 2425 2414 2418  
CONNECT 2426 2419  
CONNECT 2427 2420  
CONNECT 2428 1610 2429 2439  
CONNECT 2429 2428 2430 2436  
CONNECT 2430 2429 2431 2437  
CONNECT 2431 2430 2432 2438  
CONNECT 2432 2431 2433 2439  
CONNECT 2433 2432 2440  
CONNECT 2434 2435 2436 2441  
CONNECT 2435 2434  
CONNECT 2436 2429 2434  
CONNECT 2437 2430  
CONNECT 2438 2431  
CONNECT 2439 2428 2432  
CONNECT 2440 2433 2476  
CONNECT 2441 2434  
CONNECT 2442 1946 2443 2453  
CONNECT 2443 2442 2444 2450  
CONNECT 2444 2443 2445 2451  
CONNECT 2445 2444 2446 2452  
CONNECT 2446 2445 2447 2453  
CONNECT 2447 2446 2454  
CONNECT 2448 2449 2450 2455  
CONNECT 2449 2448  
CONNECT 2450 2443 2448  
CONNECT 2451 2444

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FIG. 53-122  
CONNECT 2453 2442 2446  
CONNECT 2454 2447 2486  
CONNECT 2455 2448  
CONNECT 2456 2328 2457 2465  
CONNECT 2457 2456 2458 2462  
CONNECT 2458 2457 2459 2463  
CONNECT 2459 2458 2460 2464  
CONNECT 2460 2459 2461 2465  
CONNECT 2461 2460  
CONNECT 2462 2457  
CONNECT 2463 2458  
CONNECT 2464 2459  
CONNECT 2465 2456 2460  
CONNECT 2466 2384 2467 2475  
CONNECT 2467 2466 2468 2472  
CONNECT 2468 2467 2469 2473  
CONNECT 2469 2468 2470 2474  
CONNECT 2470 2469 2471 2475  
CONNECT 2471 2470  
CONNECT 2472 2467  
CONNECT 2473 2468  
CONNECT 2474 2469  
CONNECT 2475 2466 2470  
CONNECT 2476 2440 2477 2485  
CONNECT 2477 2476 2478 2482  
CONNECT 2478 2477 2479 2483  
CONNECT 2479 2478 2480 2484  
CONNECT 2480 2479 2481 2485  
CONNECT 2481 2480  
CONNECT 2482 2477  
CONNECT 2483 2478  
CONNECT 2484 2479  
CONNECT 2485 2476 2480  
CONNECT 2486 2454 2487 2495  
CONNECT 2487 2486 2488 2492  
CONNECT 2488 2487 2489 2493  
CONNECT 2489 2488 2490 2494  
CONNECT 2490 2489 2491 2495  
CONNECT 2491 2490  
CONNECT 2492 2487  
CONNECT 2493 2488  
CONNECT 2494 2489  
CONNECT 2495 2486 2490  
CONNECT 2613 2612 3162  
CONNECT 3162 2613 3161  
CONNECT 3506 3505 3725  
CONNECT 3725 3506 3724  
CONNECT 4073 4072 4562  
CONNECT 4562 4073 4561  
CONNECT 4942 4941 5421  
CONNECT 5421 4942 5420  
CONNECT 5711 5710 6304  
CONNECT 6304 5711 6303  
CONNECT 6719 6718 7133  
CONNECT 7133 6719 7132  
MASTER 231 0 15 13 75 0 1 67877 4 231 75  
END

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## FIG. 54A

Detailed here is a list of all the contacts between gp120 (designed here as molecule A) and CD4 (designated here as molecule B). The model is 7s\_pb6 (from 26dec97).

## Hydrogen bonds

	donor atom		acceptor atom	distance				
A	/A0125-LEU N	B	/B1064-GLN OE1	3.71MS	-1 7.14154.7	2.78111.6	111.5	48
B	/B1029-LYS NZ	A	/A0279-ASP OD2	2.75SS	-111.18152.4	1.81157.8	148.6	131
B	/B1029-LYS NZ	A	/A0280-ASN OD1	3.16SS	-110.25102.0	2.78145.4	141.4	134
A	/A0280-ASN ND2	B	/B1033-GLN O	2.71SM	-1 7.94151.6	1.79151.4	156.3	135
B	/B1052-ASN ND2	A	/A0365-SER O	2.97SM	-1 7.55135.0	2.18100.5	108.2	198
B	/B1046-LYS N	A	/A0366-GLY O	3.31MM	-1 4.90170.1	2.32114.3	112.0	199
A	/A0368-ASP N	B	/B1044-LEU O	3.44MM	-1 5.66143.5	2.59123.5	131.5	200
B	/B1059-ARG NH2	A	/A0368-ASP OD1	2.48SS	-111.53126.4	1.75 92.2	107.9	202
B	/B1044-LEU N	A	/A0368-ASP OD2	3.32MS	-1 5.66160.6	2.36 92.8	95.9	203
B	/B1059-ARG NH1	A	/A0368-ASP OD2	2.78SS	-111.53150.6	1.86132.1	121.9	204
B	/B1042-SER OG	A	/A0427-TRP O	3.42SM	-1 5.39178.3	2.42101.0	100.7	245
B	/B1025-GLN NE2	A	/A0474-ASP OD2	3.04SS	-1 9.17117.4	2.45 96.8	111.5	267

## Van der Waals contacts

	donor atom		acceptor atom	distance				
B	/B1060-SER CA	A	/A0123-THR OG1	4.12MS	-1 5.83	-1.0-1.00	-1.0	99.7 1468
B	/B1063-ASP OD2	A	/A0123-THR O	3.97SM	-1 8.60	-1.0-1.00	-1.0	154.0 1484
B	/B1064-GLN OE1	A	/A0125-LEU N	3.71SM	-1 7.14	-1.0-1.00	-1.0	98.5 1535
B	/B1064-GLN OE1	A	/A0125-LEU CA	4.18SM	-1 7.14	-1.0-1.00	-1.0	56.9 1539
B	/B1060-SER O	A	/A0125-LEU CB	3.65MS	-1 6.24	-1.0-1.00	-1.0	54.9 1542
B	/B1064-GLN CG	A	/A0125-LEU CB	4.14SS	-1 7.14	-1.0-1.00	-1.0	113.5 1543
B	/B1064-GLN CD	A	/A0125-LEU CB	4.09SS	-1 7.14	-1.0-1.00	-1.0	101.0 1544
B	/B1064-GLN OE1	A	/A0125-LEU CB	3.58SS	-1 7.14	-1.0-1.00	-1.0	102.1 1545
B	/B1060-SER CB	A	/A0125-LEU CG	3.83SS	-1 6.24	-1.0-1.00	-1.0	62.6 1548
B	/B1060-SER C	A	/A0125-LEU CG	3.58MS	-1 6.24	-1.0-1.00	-1.0	74.4 1549
B	/B1060-SER O	A	/A0125-LEU CG	3.04MS	-1 6.24	-1.0-1.00	-1.0	69.7 1550
B	/B1061-LEU CD2	A	/A0125-LEU CG	3.72SS	-1 6.32	-1.0-1.00	-1.0	79.7 1551
B	/B1061-LEU CD2	A	/A0125-LEU CD1	3.76SS	-1 6.32	-1.0-1.00	-1.0	76.8 1554
B	/B1060-SER CA	A	/A0125-LEU CD2	3.73MS	-1 6.24	-1.0-1.00	-1.0	98.6 1556
B	/B1060-SER CB	A	/A0125-LEU CD2	3.41SS	-1 6.24	-1.0-1.00	-1.0	94.1 1557
B	/B1060-SER C	A	/A0125-LEU CD2	3.49MS	-1 6.24	-1.0-1.00	-1.0	80.8 1558
B	/B1060-SER O	A	/A0125-LEU CD2	2.89MS	-1 6.24	-1.0-1.00	-1.0	80.7 1559
B	/B1029-LYS NZ	A	/A0279-ASP CG	3.87SS	-111.18143.9	3.01125.2	21.7	4270
B	/B1027-HIS CE1	A	/A0279-ASP OD1	3.89SS	-110.91	-1.0-1.00	-1.0	115.1 4278
B	/B1029-LYS CE	A	/A0279-ASP OD2	3.86SS	-111.18	-1.0-1.00	-1.0	157.5 4288
B	/B1029-LYS NZ	A	/A0279-ASP OD2	2.75SS	-111.18152.4	1.81157.8	148.6	4289
B	/B1035-LYS CD	A	/A0280-ASN CB	3.84SS	-1 7.81	-1.0-1.00	-1.0	60.0 4321
B	/B1029-LYS CE	A	/A0280-ASN CG	4.10SS	-110.25	-1.0-1.00	-1.0	25.5 4326
B	/B1029-LYS NZ	A	/A0280-ASN CG	4.19SS	-110.25101.9	3.87121.4	28.0	4327
B	/B1033-GLN O	A	/A0280-ASN CG	3.70MS	-1 7.94	-1.0-1.00	-1.0	34.4 4328
B	/B1035-LYS CD	A	/A0280-ASN CG	3.35SS	-1 7.81	-1.0-1.00	-1.0	72.3 4329
B	/B1029-LYS CE	A	/A0280-ASN OD1	3.03SS	-110.25	-1.0-1.00	-1.0	144.3 4335
B	/B1029-LYS NZ	A	/A0280-ASN OD1	3.16SS	-110.25102.0	2.78145.4	141.4	4336
B	/B1033-GLN O	A	/A0280-ASN OD1	3.89MS	-1 7.94	-1.0-1.00	-1.0	71.8 4337
B	/B1035-LYS CG	A	/A0280-ASN OD1	3.77SS	-1 7.81	-1.0-1.00	-1.0	105.2 4338
B	/B1035-LYS CD	A	/A0280-ASN OD1	3.20SS	-1 7.81	-1.0-1.00	-1.0	86.0 4339
B	/B1035-LYS CE	A	/A0280-ASN OD1	4.11SS	-1 7.81	-1.0-1.00	-1.0	87.5 4340
B	/B1033-GLN CB	A	/A0280-ASN ND2	4.13SS	-1 7.94	-1.0-1.00	-1.0	132.0 4343
B	/B1033-GLN C	A	/A0280-ASN ND2	3.87MS	-1 7.94	-1.0-1.00	-1.0	134.5 4344
B	/B1033-GLN O	A	/A0280-ASN ND2	2.71MS	-1 7.94	-1.0-1.00	-1.0	129.6 4345
B	/B1035-LYS CD	A	/A0280-ASN ND2	3.85SS	-1 7.81	-1.0-1.00	-1.0	58.2 4346
B	/B1035-LYS CD	A	/A0280-ASN C	3.83SM	-1 7.81	-1.0-1.00	-1.0	75.4 4352
B	/B1035-LYS CE	A	/A0280-ASN C	3.57SM	-1 7.81	-1.0-1.00	-1.0	53.2 4353

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FIG. 54B

B	/B1035-LYS CE A	/A0280-ASN O	3.00SM	-1	7.81	-1.0	-1.00	-1.0	107.7	4362
B	/B1035-LYS CD A	/A0281-ALA N	4.03SM	-1	7.00	-1.0	-1.00	-1.0	71.7	4365
B	/B1035-LYS CE A	/A0281-ALA N	3.94SM	-1	7.00	-1.0	-1.00	-1.0	64.4	4366
B	/B1035-LYS CD A	/A0281-ALA CA	4.16SM	-1	7.00	-1.0	-1.00	-1.0	74.8	4368
B	/B1035-LYS CE A	/A0281-ALA CA	3.80SM	-1	7.00	-1.0	-1.00	-1.0	84.3	4369
B	/B1027-HIS CG A	/A0281-ALA CB	3.57SS	-1	7.00	-1.0	-1.00	-1.0	147.8	4372
B	/B1027-HIS CD2 A	/A0281-ALA CB	3.64SS	-1	7.00	-1.0	-1.00	-1.0	139.6	4373
B	/B1027-HIS ND1 A	/A0281-ALA CB	3.31SS	-1	7.00	61.5	3.67160.4	168.7	4374	4374
B	/B1027-HIS CE1 A	/A0281-ALA CB	3.24SS	-1	7.00	-1.0	-1.00	-1.0	165.4	4375
B	/B1027-HIS NE2 A	/A0281-ALA CB	3.44SS	-1	7.00	56.4	3.89134.4	146.1	4376	4376
B	/B1029-LYS CE A	/A0281-ALA CB	4.02SS	-1	9.11	-1.0	-1.00	-1.0	112.9	4377
B	/B1029-LYS NZ A	/A0281-ALA CB	4.09SS	-1	9.11125.9	3.41105.0	112.6	4378	4378	4378
B	/B1040-GLN CD A	/A0283-THR OG1	3.78SS	-1	9.11	-1.0	-1.00	-1.0	172.3	4419
B	/B1040-GLN OE1 A	/A0283-THR OG1	3.38SS	-1	9.11	-1.0	-1.00	-1.0	164.0	4420
B	/B1040-GLN NE2 A	/A0283-THR OG1	3.67SS	-1	9.11110.8	3.19139.9	152.1	4421	4421	4421
B	/B1046-LYS O A	/A0365-SER CA	3.92MM	-1	5.83	-1.0	-1.00	-1.0	40.5	6411
B	/B1046-LYS C A	/A0365-SER CB	3.76MS	-1	5.83	-1.0	-1.00	-1.0	111.4	6414
B	/B1046-LYS O A	/A0365-SER CB	2.93MS	-1	5.83	-1.0	-1.00	-1.0	110.5	6415
B	/B1047-GLY N A	/A0365-SER CB	4.10MS	-1	5.10	20.9	5.02146.7	98.6	6416	6416
B	/B1047-GLY CA A	/A0365-SER CB	3.62MS	-1	5.10	-1.0	-1.00	-1.0	79.3	6417
B	/B1047-GLY C A	/A0365-SER CB	3.24MS	-1	5.10	-1.0	-1.00	-1.0	80.2	6418
B	/B1047-GLY O A	/A0365-SER CB	3.21MS	-1	5.10	-1.0	-1.00	-1.0	100.1	6419
B	/B1048-PRO N A	/A0365-SER CB	3.71MS	-1	5.39	-1.0	-1.00	-1.0	63.0	6420
B	/B1052-ASN ND2 A	/A0365-SER CB	3.93SS	-1	7.55106.8	3.52156.0	91.9	6421	6421	6421
B	/B1046-LYS O A	/A0365-SER OG	3.67MS	-1	5.83	-1.0	-1.00	-1.0	48.4	6428
B	/B1047-GLY CA A	/A0365-SER OG	3.64MS	-1	5.10	-1.0	-1.00	-1.0	78.2	6429
B	/B1047-GLY C A	/A0365-SER OG	3.31MS	-1	5.10	-1.0	-1.00	-1.0	74.9	6430
B	/B1047-GLY O A	/A0365-SER OG	3.73MS	-1	5.10	-1.0	-1.00	-1.0	58.0	6431
B	/B1048-PRO N A	/A0365-SER OG	3.32MS	-1	5.39	-1.0	-1.00	-1.0	94.6	6432
B	/B1048-PRO CD A	/A0365-SER OG	3.43SS	-1	5.39	-1.0	-1.00	-1.0	118.0	6433
B	/B1048-PRO CA A	/A0365-SER OG	3.90MS	-1	5.39	-1.0	-1.00	-1.0	95.1	6434
B	/B1048-PRO CG A	/A0365-SER OG	3.38SS	-1	5.39	-1.0	-1.00	-1.0	132.0	6435
B	/B1046-LYS O A	/A0365-SER C	3.93MM	-1	5.83	-1.0	-1.00	-1.0	65.9	6438
B	/B1052-ASN ND2 A	/A0365-SER C	3.56SM	-1	7.55144.7	2.70115.1	52.5	6439	6439	6439
B	/B1052-ASN CG A	/A0365-SER O	3.69SM	-1	7.55	-1.0	-1.00	-1.0	127.2	6442
B	/B1052-ASN OD1 A	/A0365-SER O	3.71SM	-1	7.55	-1.0	-1.00	-1.0	139.5	6443
B	/B1052-ASN ND2 A	/A0365-SER O	2.97SM	-1	7.55135.0	2.18100.5	108.2	6444	6444	6444
B	/B1046-LYS O A	/A0366-GLY N	3.60MM	-1	4.90	-1.0	-1.00	-1.0	94.4	6447
B	/B1052-ASN ND2 A	/A0366-GLY N	4.20SM	-1	7.21162.2	3.24	83.1	53.0	6448	6448
B	/B1046-LYS N A	/A0366-GLY C	3.94MM	-1	4.90150.1	3.04116.2	51.1	6454	6454	6454
B	/B1046-LYS CB A	/A0366-GLY C	4.06SM	-1	4.90	-1.0	-1.00	-1.0	84.8	6455
B	/B1045-THR CA A	/A0366-GLY O	4.05MM	-1	6.16	-1.0	-1.00	-1.0	130.3	6459
B	/B1045-THR C A	/A0366-GLY O	4.19MM	-1	6.16	-1.0	-1.00	-1.0	119.9	6460
B	/B1046-LYS N A	/A0366-GLY O	3.31MM	-1	4.90170.1	2.32114.3	112.0	6461	6461	6461
B	/B1046-LYS CA A	/A0366-GLY O	4.14MM	-1	4.90	-1.0	-1.00	-1.0	99.2	6462
B	/B1046-LYS CB A	/A0366-GLY O	4.13SM	-1	4.90	-1.0	-1.00	-1.0	77.9	6463
B	/B1046-LYS O A	/A0366-GLY O	3.67MM	-1	4.90	-1.0	-1.00	-1.0	110.6	6464
B	/B1044-LEU O A	/A0367-GLY CA	3.70MM	-1	5.29	-1.0	-1.00	-1.0	92.0	6470
B	/B1044-LEU O A	/A0367-GLY C	4.04MM	-1	5.29	-1.0	-1.00	-1.0	54.3	6477
B	/B1044-LEU O A	/A0368-ASP N	3.44MM	-1	5.66	-1.0	-1.00	-1.0	107.4	6488
B	/B1043-PHE CB A	/A0368-ASP CB	4.00SS	-1	5.83	-1.0	-1.00	-1.0	80.4	6500
B	/B1043-PHE CD1 A	/A0368-ASP CB	3.89SS	-1	5.83	-1.0	-1.00	-1.0	78.3	6501
B	/B1043-PHE CA A	/A0368-ASP CG	4.07MS	-1	5.83	-1.0	-1.00	-1.0	72.0	6507
B	/B1043-PHE CB A	/A0368-ASP CG	4.03SS	-1	5.83	-1.0	-1.00	-1.0	77.9	6508
B	/B1043-PHE CD1 A	/A0368-ASP CG	3.87SS	-1	5.83	-1.0	-1.00	-1.0	49.1	6509
B	/B1044-LEU N A	/A0368-ASP CG	3.67MS	-1	5.66157.3	2.72110.6	64.2	6510	6510	6510
B	/B1059-ARG CZ A	/A0368-ASP CG	3.76SS	-111.53	-1.0	-1.00	-1.0	60.7	6511	6511
B	/B1059-ARG NH1 A	/A0368-ASP CG	3.60SS	-111.53131.6	2.86148.6	40.9	6512	6512	6512	6512
B	/B1059-ARG NH2 A	/A0368-ASP CG	3.10SS	-111.53150.5	2.19148.5	49.6	6513	6513	6513	6513
B	/B1043-PHE CA A	/A0368-ASP OD1	3.88MS	-1	5.83	-1.0	-1.00	-1.0	90.2	6519
B	/B1043-PHE CB A	/A0368-ASP OD1	3.96SS	-1	5.83	-1.0	-1.00	-1.0	84.2	6520
B	/B1043-PHE CG A	/A0368-ASP OD1	4.04SS	-1	5.83	-1.0	-1.00	-1.0	100.3	6521
B	/B1043-PHE CD1 A	/A0368-ASP OD1	3.20SS	-1	5.83	-1.0	-1.00	-1.0	113.8	6522
B	/B1043-PHE CE1 A	/A0368-ASP OD1	4.08SS	-1	5.83	-1.0	-1.00	-1.0	125.2	6523
B	/B1044-LEU N A	/A0368-ASP OD1	4.08MS	-1	5.66152.1	3.17	57.9	62.0	6524	6524
B	/B1059-ARG CZ A	/A0368-ASP OD1	3.37SS	-111.53	-1.0	-1.00	-1.0	98.4	6525	6525

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FIG. 54C

B	/B1059-ARG NH2 A	/A0368-ASP OD1	2.48SS	-111.53126.4	1.75	92.2	107.9	6527
B	/B1044-LEU N A	/A0368-ASP OD2	3.32MS	-1 5.66160.6	2.36	92.8	95.9	6528
B	/B1044-LEU CA A	/A0368-ASP OD2	3.92MS	-1 5.66 -1.0-1.00	-1.0	114.9		6529
B	/B1044-LEU CB A	/A0368-ASP OD2	3.50SS	-1 5.66 -1.0-1.00	-1.0	137.6		6530
B	/B1044-LEU O A	/A0368-ASP OD2	4.02MS	-1 5.66 -1.0-1.00	-1.0	98.2		6531
B	/B1059-ARG CZ A	/A0368-ASP OD2	3.33SS	-111.53 -1.0-1.00	-1.0	100.1		6532
B	/B1059-ARG NH1 A	/A0368-ASP OD2	2.78SS	-111.53150.6	1.86132.1	121.9		6533
B	/B1059-ARG NH2 A	/A0368-ASP OD2	3.06SS	-111.53135.8	2.26	70.4	80.0	6534
B	/B1043-PHE CD1 A	/A0370-GLU CB	4.00SS	-1 7.48 -1.0-1.00	-1.0	86.6		6631
B	/B1043-PHE CE1 A	/A0370-GLU CB	3.62SS	-1 7.48 -1.0-1.00	-1.0	71.9		6632
B	/B1043-PHE CE2 A	/A0370-GLU CB	4.16SS	-1 7.48 -1.0-1.00	-1.0	97.5		6633
B	/B1043-PHE CZ A	/A0370-GLU CB	3.71SS	-1 7.48 -1.0-1.00	-1.0	78.5		6634
B	/B1043-PHE CD1 A	/A0370-GLU CG	4.20SS	-1 7.48 -1.0-1.00	-1.0	72.1		6640
B	/B1043-PHE CE1 A	/A0370-GLU CG	3.46SS	-1 7.48 -1.0-1.00	-1.0	79.0		6641
B	/B1043-PHE CZ A	/A0370-GLU CG	3.72SS	-1 7.48 -1.0-1.00	-1.0	77.7		6642
B	/B1043-PHE CD1 A	/A0370-GLU CD	4.02SS	-1 7.48 -1.0-1.00	-1.0	54.3		6651
B	/B1043-PHE CE1 A	/A0370-GLU CD	3.51SS	-1 7.48 -1.0-1.00	-1.0	73.6		6652
B	/B1043-PHE CD1 A	/A0370-GLU OE2	3.44SS	-1 7.48 -1.0-1.00	-1.0	108.6		6668
B	/B1043-PHE CE1 A	/A0370-GLU OE2	3.38SS	-1 7.48 -1.0-1.00	-1.0	85.6		6669
B	/B1044-LEU O A	/A0371-ILE CB	4.04MS	-1 7.62 -1.0-1.00	-1.0	71.8		6695
B	/B1044-LEU O A	/A0371-ILE CG2	4.02MS	-1 7.62 -1.0-1.00	-1.0	80.1		6700
B	/B1045-THR CG2 A	/A0371-ILE CG2	3.79SS	-1 7.07 -1.0-1.00	-1.0	113.2		6701
B	/B1043-PHE CB A	/A0371-ILE CG1	3.23SS	-1 6.78 -1.0-1.00	-1.0	100.0		6704
B	/B1043-PHE CG A	/A0371-ILE CG1	3.83SS	-1 6.78 -1.0-1.00	-1.0	86.6		6705
B	/B1043-PHE CD2 A	/A0371-ILE CG1	4.18SS	-1 6.78 -1.0-1.00	-1.0	67.3		6706
B	/B1044-LEU O A	/A0371-ILE CG1	3.85MS	-1 7.62 -1.0-1.00	-1.0	86.2		6707
B	/B1043-PHE CB A	/A0371-ILE CD1	3.79SS	-16.78 -1.0-1.00	-1.0	56.9		6713
B	/B1043-PHE CG A	/A0371-ILE CD1	4.03SS	-16.78 -1.0-1.00	-1.0	71.4		6714
B	/B1043-PHE CD2 A	/A0371-ILE CD1	3.86SS	-1 6.78 -1.0-1.00	-1.0	91.5		6715
B	/B1043-PHE CE1 A	/A0425-ASN CA	4.18SM	-1 7.21 -1.0-1.00	-1.0	52.7		7996
B	/B1043-PHE CD1 A	/A0425-ASN CB	3.83SS	-1 7.21 -1.0-1.00	-1.0	118.6		8000
B	/B1043-PHE CE1 A	/A0425-ASN CB	3.47SS	-1 7.21 -1.0-1.00	-1.0	106.7		8001
B	/B1043-PHE CE1 A	/A0425-ASN C	3.63SM	-1 7.21 -1.0-1.00	-1.0	55.5		8013
B	/B1043-PHE CZ A	/A0425-ASN C	4.17SM	-1 7.21 -1.0-1.00	-1.0	43.8		8014
B	/B1043-PHE CE1 A	/A0425-ASN O	3.10SM	-1 7.21 -1.0-1.00	-1.0	105.3		8019
B	/B1043-PHE CZ A	/A0425-ASN O	3.38SM	-1 7.21 -1.0-1.00	-1.0	121.5		8020
B	/B1042-SER CB A	/A0426-MET C	4.18SM	-1 6.71 -1.0-1.00	-1.0	26.9		8055
B	/B1043-PHE CE1 A	/A0426-MET C	3.99SM	-1 7.81 -1.0-1.00	-1.0	60.1		8056
B	/B1043-PHE CZ A	/A0426-MET C	3.67SM	-1 7.81 -1.0-1.00	-1.0	71.0		8057
B	/B1042-SER CB A	/A0426-MET O	3.13SM	-1 6.71 -1.0-1.00	-1.0	142.8		8063
B	/B1042-SER OG A	/A0426-MET O	3.82SM	-1 6.71106.4	3.42108.3	122.6		8064
B	/B1043-PHE CE1 A	/A0426-MET O	3.54SM	-1 7.81 -1.0-1.00	-1.0	102.2		8065
B	/B1043-PHE CE2 A	/A0426-MET O	4.12SM	-1 7.81 -1.0-1.00	-1.0	97.5		8066
B	/B1043-PHE CZ A	/A0426-MET O	3.47SM	-1 7.81 -1.0-1.00	-1.0	89.3		8067
B	/B1043-PHE CZ A	/A0427-TRP N	3.74SM	-1 7.00 -1.0-1.00	-1.0	76.0		8075
B	/B1043-PHE CE2 A	/A0427-TRP CA	3.72SM	-1 7.00 -1.0-1.00	-1.0	73.6		8080
B	/B1043-PHE CZ A	/A0427-TRP CA	3.67SM	-1 7.00 -1.0-1.00	-1.0	80.7		8081
B	/B1043-PHE CE2 A	/A0427-TRP CB	3.61SS	-1 7.00 -1.0-1.00	-1.0	82.2		8088
B	/B1043-PHE CZ A	/A0427-TRP CB	3.75SS	-1 7.00 -1.0-1.00	-1.0	75.4		8089
B	/B1042-SER OG A	/A0427-TRP C	3.84SM	-1 5.39165.6	2.86109.0	61.0		8137
B	/B1042-SER CB A	/A0427-TRP O	4.10SM	-1 5.39 -1.0-1.00	-1.0	91.1		8142
B	/B1042-SER OG A	/A0427-TRP O	3.42SM	-1 5.39178.3	2.42101.0	100.7		8143
B	/B1042-SER OG A	/A0428-GLN C	3.93SM	-1 7.00144.1	3.08111.8	63.1		8161
B	/B1042-SER OG A	/A0428-GLN O	4.11SM	-1 7.00124.7	3.45	62.8		8165
B	/B1042-SER OG A	/A0429-LYS N	3.53SM	-1 5.57156.5	2.59101.3	69.4		8169
B	/B1042-SER OG A	/A0429-LYS CA	3.31SM	-1 5.57151.2	2.40163.3	66.5		8172
B	/B1042-SER CB A	/A0429-LYS C	3.65SM	-1 5.57 -1.0-1.00	-1.0	72.5		8185
B	/B1042-SER OG A	/A0429-LYS C	3.05SM	-1 5.57171.0	2.05	95.9	86.1	8186
B	/B1042-SER CB A	/A0429-LYS O	3.49SM	-1 5.57 -1.0-1.00	-1.0	87.7		8191
B	/B1042-SER OG A	/A0429-LYS O	3.23SM	-1 5.57149.1	2.33	63.9	70.2	8192
B	/B1042-SER CB A	/A0430-VAL N	3.88SM	-1 4.80 -1.0-1.00	-1.0	70.4		8197
B	/B1042-SER OG A	/A0430-VAL N	3.43SM	-1 4.80162.4	2.47109.9	62.1		8198
B	/B1042-SER CB A	/A0430-VAL CA	4.00SM	-1 4.80 -1.0-1.00	-1.0	74.7		8200
B	/B1042-SER OG A	/A0430-VAL CA	4.06SM	-1 4.80137.8	3.27139.6	54.7		8201
B	/B1059-ARG CB A	/A0430-VAL CG1	3.68SS	-1 6.78 -1.0-1.00	-1.0	135.4		8207
B	/B1059-ARG C A	/A0430-VAL CG1	4.13MS	-1 6.78 -1.0-1.00	-1.0	121.7		8208

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## FIG. 54D

B	/B1042-SER CA A	/A0430-VAL CG2	3.98MS	-1 4.80	-1.0-1.00	-1.0	127.6	8211
B	/B1042-SER CB A	/A0430-VAL CG2	4.01SS	-1 4.80	-1.0-1.00	-1.0	106.6	8212
B	/B1042-SER O A	/A0430-VAL CG2	3.94MS	-1 4.80	-1.0-1.00	-1.0	115.4	8213
B	/B1062-TRP CE3 A	/A0430-VAL CG2	3.38SS	-1 7.87	-1.0-1.00	-1.0	142.7	8214
B	/B1062-TRP CZ3 A	/A0430-VAL CG2	3.96SS	-1 7.87	-1.0-1.00	-1.0	143.2	8215
B	/B1035-LYS CE A	/A0455-THR CG2	3.99SS	-110.54	-1.0-1.00	-1.0	133.1	8736
B	/B1035-LYS NZ A	/A0455-THR CG2	3.54SS	-110.54	135.4 2.74	136.5	144.6	8737
B	/B1035-LYS CD A	/A0456-ARG O	4.17SM	-1 9.59	-1.0-1.00	-1.0	155.2	8795
B	/B1035-LYS CE A	/A0456-ARG O	3.84SM	-1 9.59	-1.0-1.00	-1.0	142.6	8796
B	/B1048-PRO CG A	/A0457-ASP CG	3.74SS	-1 7.35	-1.0-1.00	-1.0	66.0	8817
B	/B1048-PRO CG A	/A0457-ASP OD1	3.75SS	-1 7.35	-1.0-1.00	-1.0	80.0	8824
B	/B1048-PRO CG A	/A0457-ASP OD2	3.43SS	-1 7.35	-1.0-1.00	-1.0	94.6	8832
B	/B1034-ILE CD1 A	/A0458-GLY C	4.05SM	-1 5.29	-1.0-1.00	-1.0	72.8	8847
B	/B1034-ILE CD1 A	/A0458-GLY O	3.87SM	-1 5.29	-1.0-1.00	-1.0	89.5	8854
B	/B1032-ASN O A	/A0459-GLY N	3.61MM	-1 5.10	-1.0-1.00	-1.0	58.0	8858
B	/B1033-GLN O A	/A0459-GLY N	4.14MM	-1 5.10	-1.0-1.00	-1.0	98.1	8859
B	/B1034-ILE CD1 A	/A0459-GLY N	4.05SM	-1 5.29	-1.0-1.00	-1.0	69.7	8860
B	/B1032-ASN O A	/A0459-GLY CA	3.09MM	-1 5.10	-1.0-1.00	-1.0	98.6	8862
B	/B1034-ILE CD1 A	/A0459-GLY CA	3.80SM	-1 5.29	-1.0-1.00	-1.0	89.3	8863
B	/B1048-PRO CG A	/A0469-ARG NE	3.83SS	-110.34	-1.0-1.00	-1.0	78.9	9135
B	/B1048-PRO CG A	/A0469-ARG CZ	3.80SS	-110.34	-1.0-1.00	-1.0	58.9	9136
B	/B1048-PRO CB A	/A0469-ARG NH2	3.73SS	-110.34	-1.0-1.00	-1.0	119.1	9137
B	/B1048-PRO CG A	/A0469-ARG NH2	3.32SS	-110.34	-1.0-1.00	-1.0	101.1	9138
B	/B1040-GLN CB A	/A0472-GLY O	3.40SM	-1 6.86	-1.0-1.00	-1.0	128.3	9178
B	/B1040-GLN CG A	/A0472-GLY O	3.48SM	-1 6.86	-1.0-1.00	-1.0	136.2	9179
B	/B1040-GLN CD A	/A0472-GLY O	4.14SM	-1 6.86	-1.0-1.00	-1.0	117.0	9180
B	/B1040-GLN NE2 A	/A0472-GLY O	4.00SM	-1 6.86	120.2 3.40	92.5	99.1	9181
B	/B1040-GLN CB A	/A0473-GLY CA	3.86SM	-1 4.58	-1.0-1.00	-1.0	92.8	9186
B	/B1040-GLN O A	/A0473-GLY CA	3.30MM	-1 4.58	-1.0-1.00	-1.0	65.4	9187
B	/B1043-PHE CD2 A	/A0473-GLY CA	3.87SM	-1 6.00	-1.0-1.00	-1.0	96.6	9188
B	/B1040-GLN C A	/A0473-GLY C	3.79MM	-1 4.58	-1.0-1.00	-1.0	79.1	9193
B	/B1040-GLN O A	/A0473-GLY C	3.00MM	-1 4.58	-1.0-1.00	-1.0	87.0	9194
B	/B1040-GLN C A	/A0473-GLY O	4.09MM	-1 4.58	-1.0-1.00	-1.0	67.4	9201
B	/B1040-GLN O A	/A0473-GLY O	3.18MM	-1 4.58	-1.0-1.00	-1.0	70.2	9202
B	/B1043-PHE CD2 A	/A0473-GLY O	3.90SM	-1 6.00	-1.0-1.00	-1.0	101.1	9203
B	/B1043-PHE CE2 A	/A0473-GLY O	4.05SM	-1 6.00	-1.0-1.00	-1.0	115.8	9204
B	/B1040-GLN CB A	/A0474-ASP N	4.09SM	-1 4.90	-1.0-1.00	-1.0	86.0	9208
B	/B1040-GLN NE2 A	/A0474-ASP N	3.62SM	-1 4.90	153.2 2.70	120.8	103.2	9209
B	/B1040-GLN C A	/A0474-ASP N	3.78MM	-1 4.90	-1.0-1.00	-1.0	80.7	9210
B	/B1040-GLN O A	/A0474-ASP N	3.39MM	-1 4.90	-1.0-1.00	-1.0	61.8	9211
B	/B1040-GLN NE2 A	/A0474-ASP CA	4.20SM	-1 4.90	131.5 3.47	129.6	55.0	9216
B	/B1040-GLN C A	/A0474-ASP CA	4.17MM	-1 4.90	-1.0-1.00	-1.0	64.5	9217
B	/B1040-GLN O A	/A0474-ASP CA	4.01MM	-1 4.90	-1.0-1.00	-1.0	54.9	9218
B	/B1025-GLN NE2 A	/A0474-ASP CB	3.76SS	-1 9.17	131.5 3.02	122.7	75.7	9222
B	/B1040-GLN NE2 A	/A0474-ASP CB	3.55SS	-1 4.90	105.3 3.15	148.9	104.4	9223
B	/B1025-GLN NE2 A	/A0474-ASP CG	3.69SS	-1 9.17	138.5 2.88	133.3	50.1	9232
B	/B1025-GLN CD A	/A0474-ASP OD2	4.09SS	-1 9.17	-1.0-1.00	-1.0	118.2	9246
B	/B1025-GLN NE2 A	/A0474-ASP OD2	3.04SS	-1 9.17	117.4 2.45	96.8	111.5	9247
B	/B1040-GLN NE2 A	/A0477-ASP OD2	4.10SS	-1 9.49	144.4 3.25	134.2	134.4	9372

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## FIG. 55A

Detailed here is a list of all the contacts between gp120 (designed here as molecule A) and the Fab 17b (the light chain is designated here as molecule C; the heavy chain is designated here as molecule D). The model is 7s\_pb6 (from 26dec97).

## Hydrogen bonds

	donor atom	acceptor atom	distance	
C	/C2094-TRP NE1 A	/A0119-CYS SG	3.37SS -110.05119.2 2.76115.1 124.6	40
A	/A0121-LYS NZ D	/D3055-LEU O	2.64SM -1 8.31111.1 2.10 96.1 115.1	43
A	/A0202-THR OG1 D	/D3059-HIS NE2	2.76SS -1 8.60179.9 1.76136.3 107.3	53
D	/D3059-HIS NE2 A	/A0202-THR OG1	2.76SS -1 8.60132.4 1.99103.7 110.1	54
A	/A0419-ARG NH1 D	/D3106-GLU OE1	2.76SS -1 8.89138.6 1.93139.5 131.5	236
A	/A0419-ARG NH2 D	/D3106-GLU OE1	2.94SS -1 8.89131.6 2.18122.8 121.6	237
A	/A0422-GLN N D	/D3107-GLY O	2.84MM -1 5.48155.6 1.90126.3 131.0	238
D	/D3109-TYR N A	/A0422-GLN OE1	2.73MS -1 6.08159.9 1.77161.2 156.1	239
A	/A0423-ILE N D	/D3107-GLY O	2.89MM -1 4.58165.6 1.91136.9 141.7	241

## Van der Waals contacts

	donor atom	acceptor atom	distance	
C	/C2094-TRP CE2 A	/A0119-CYS SG	4.08SS -110.05 -1.0-1.00 -1.0 115.4	1319
C	/C2094-TRP CD1 A	/A0119-CYS SG	4.16SS -110.05 -1.0-1.00 -1.0 141.5	1320
C	/C2094-TRP NE1 A	/A0119-CYS SG	3.37SS -110.05119.2 2.76115.1 124.6	1321
C	/C2094-TRP CE2 A	/A0202-THR CG2	4.19SS -1 8.37 -1.0-1.00 -1.0 149.8	1802
C	/C2094-TRP NE1 A	/A0202-THR CG2	3.48SS -1 8.37118.7 2.89131.0 145.6	1803
C	/C2095-PRO CA A	/A0202-THR CG2	4.14MS -1 6.48 -1.0-1.00 -1.0 148.5	1804
C	/C2095-PRO CB A	/A0202-THR CG2	3.65SS -1 6.48 -1.0-1.00 -1.0 127.3	1805
C	/C2095-PRO CG A	/A0202-THR CG2	3.31SS -1 6.48 -1.0-1.00 -1.0 116.7	1806
C	/C2095-PRO CG A	/A0202-THR O	4.06SM -1 6.48 -1.0-1.00 -1.0 113.1	1817
C	/C2094-TRP CD1 A	/A0203-GLN O	3.41SM -1 8.00 -1.0-1.00 -1.0 135.7	1841
C	/C2094-TRP NE1 A	/A0203-GLN O	3.49SM -1 8.00112.3 2.98147.4 149.2	1842
C	/C2094-TRP CD1 A	/A0205-CYS N	4.12SM -1 7.42 -1.0-1.00 -1.0 110.8	1865
C	/C2094-TRP CZ2 A	/A0434-MET CE	3.88SS -112.65 -1.0-1.00 -1.0 160.1	8276
C	/C2094-TRP CH2 A	/A0434-MET CE	3.86SS -112.65 -1.0-1.00 -1.0 140.7	8277
D	/D3055-LEU CB A	/A0121-LYS CD	4.13SS -1 8.31 -1.0-1.00 -1.0 79.8	1380
D	/D3055-LEU O A	/A0121-LYS CD	3.87MS -1 8.31 -1.0-1.00 -1.0 77.5	1381
D	/D3057-VAL CG1 A	/A0121-LYS CD	3.85SS -1 9.06 -1.0-1.00 -1.0 109.0	1382
D	/D3055-LEU CB A	/A0121-LYS CE	4.14SS -1 8.31 -1.0-1.00 -1.0 57.4	1383
D	/D3055-LEU CG A	/A0121-LYS CE	4.09SS -1 8.31 -1.0-1.00 -1.0 74.0	1384
D	/D3055-LEU O A	/A0121-LYS CE	3.83MS -1 8.31 -1.0-1.00 -1.0 29.5	1385
D	/D3055-LEU CA A	/A0121-LYS NZ	3.30MS -1 8.31 -1.0-1.00 -1.0 126.8	1386
D	/D3055-LEU CB A	/A0121-LYS NZ	3.56SS -1 8.31 -1.0-1.00 -1.0 102.0	1387
D	/D3055-LEU CG A	/A0121-LYS NZ	3.94SS -1 8.31 -1.0-1.00 -1.0 84.8	1388
D	/D3055-LEU C A	/A0121-LYS NZ	3.36MS -1 8.31 -1.0-1.00 -1.0 136.7	1389
D	/D3055-LEU O A	/A0121-LYS NZ	2.64MS -1 8.31 -1.0-1.00 -1.0 134.4	1390
D	/D3057-VAL CG1 A	/A0200-VAL CB	3.75SS -1 7.35 -1.0-1.00 -1.0 71.3	1745
D	/D3057-VAL CG1 A	/A0200-VAL CG1	3.57SS -1 7.35 -1.0-1.00 -1.0 84.9	1747
D	/D3059-HIS CD2 A	/A0202-THR CB	3.94SS -1 8.60 -1.0-1.00 -1.0 56.4	1792
D	/D3059-HIS NE2 A	/A0202-THR CB	3.52SS -1 8.60138.2 2.71119.7 47.4	1793
D	/D3059-HIS CD2 A	/A0202-THR OG1	3.44SS -1 8.60 -1.0-1.00 -1.0 99.6	1796
D	/D3059-HIS NE2 A	/A0202-THR OG1	2.76SS -1 8.60132.4 1.99103.7 110.1	1797
D	/D3059-HIS CE1 A	/A0202-THR OG1	3.82SS -1 8.60 -1.0-1.00 -1.0 122.6	1798
D	/D3059-HIS CD2 A	/A0202-THR CG2	3.35SS -1 8.60 -1.0-1.00 -1.0 101.3	1807
D	/D3059-HIS NE2 A	/A0202-THR CG2	3.12SS -1 8.60121.9 2.47 81.9 92.2	1808
D	/D3106-GLU O A	/A0419-ARG CD	4.00MS -1 8.89 -1.0-1.00 -1.0 68.2	7757
D	/D3106-GLU O A	/A0419-ARG NE	3.72MS -1 8.89 -1.0-1.00 -1.0 90.2	7758
D	/D3106-GLU CB A	/A0419-ARG CZ	3.76SS -1 8.89 -1.0-1.00 -1.0 79.6	7759
D	/D3106-GLU CD A	/A0419-ARG CZ	4.09SS -1 8.89 -1.0-1.00 -1.0 64.2	7760
-	/D3106-GLU CD A	/A0419-ARG CZ	3.22SS -1 8.89 -1.0-1.00 -1.0 57.6	7761



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FIG. 55B

D	/D3106-GLU CB A	/A0419-ARG NH1	3.79SS	-1	8.89	-1.0	-1.00	-1.0	78.6	7763
D	/D3106-GLU CG A	/A0419-ARG NH1	3.90SS	-1	8.89	-1.0	-1.00	-1.0	98.1	7764
D	/D3106-GLU CD A	/A0419-ARG NH1	3.71SS	-1	8.89	-1.0	-1.00	-1.0	97.0	7765
D	/D3106-GLU OE1 A	/A0419-ARG NH1	2.76SS	-1	8.89	-1.0	-1.00	-1.0	98.4	7766
D	/D3106-GLU CB A	/A0419-ARG NH2	3.76SS	-1	8.89	-1.0	-1.00	-1.0	80.0	7767
D	/D3106-GLU CD A	/A0419-ARG NH2	3.75SS	-1	8.89	-1.0	-1.00	-1.0	95.1	7768
D	/D3106-GLU OE1 A	/A0419-ARG NH2	2.94SS	-1	8.89	-1.0	-1.00	-1.0	90.3	7769
D	/D3108-GLU CB A	/A0419-ARG NH2	3.48SS	-1	8.89	-1.0	-1.00	-1.0	119.9	7770
D	/D3108-GLU CG A	/A0419-ARG NH2	4.07SS	-1	8.89	-1.0	-1.00	-1.0	131.1	7771
D	/D3108-GLU CD A	/A0419-ARG NH2	3.54SS	-1	8.89	-1.0	-1.00	-1.0	144.5	7772
D	/D3108-GLU OE1 A	/A0419-ARG NH2	3.89SS	-1	8.89	-1.0	-1.00	-1.0	163.1	7773
D	/D3108-GLU OE2 A	/A0419-ARG NH2	3.40SS	-1	8.89	-1.0	-1.00	-1.0	130.5	7774
D	/D3107-GLY C A	/A0421-LYS CA	4.19MM	-1	4.58	-1.0	-1.00	-1.0	72.9	7812
D	/D3107-GLY O A	/A0421-LYS CA	3.94MM	-1	4.58	-1.0	-1.00	-1.0	74.7	7813
D	/D3106-GLU O A	/A0421-LYS CB	4.03MS	-1	7.00	-1.0	-1.00	-1.0	45.2	7817
D	/D3107-GLY CA A	/A0421-LYS CB	3.94MS	-1	4.58	-1.0	-1.00	-1.0	83.7	7818
D	/D3107-GLY C A	/A0421-LYS CB	4.02MS	-1	4.58	-1.0	-1.00	-1.0	85.8	7819
D	/D3107-GLY O A	/A0421-LYS CB	3.98MS	-1	4.58	-1.0	-1.00	-1.0	77.1	7820
D	/D3106-GLU C A	/A0421-LYS CG	4.17MS	-1	7.00	-1.0	-1.00	-1.0	66.3	7823
D	/D3106-GLU O A	/A0421-LYS CG	3.16MS	-1	7.00	-1.0	-1.00	-1.0	72.9	7824
D	/D3107-GLY CA A	/A0421-LYS CG	4.06MS	-1	4.58	-1.0	-1.00	-1.0	73.7	7825
D	/D3106-GLU C A	/A0421-LYS CD	3.82MS	-1	7.00	-1.0	-1.00	-1.0	79.4	7826
D	/D3106-GLU O A	/A0421-LYS CD	3.07MS	-1	7.00	-1.0	-1.00	-1.0	75.7	7827
D	/D3107-GLY CA A	/A0421-LYS CD	3.91MS	-1	4.58	-1.0	-1.00	-1.0	84.5	7828
D	/D3106-GLU C A	/A0421-LYS CE	3.85MS	-1	7.00	-1.0	-1.00	-1.0	77.8	7829
D	/D3106-GLU O A	/A0421-LYS CE	3.07MS	-1	7.00	-1.0	-1.00	-1.0	75.7	7830
D	/D3106-GLU C A	/A0421-LYS NZ	3.87MS	-1	7.00	-1.0	-1.00	-1.0	78.2	7831
D	/D3106-GLU O A	/A0421-LYS NZ	3.53MS	-1	7.00	-1.0	-1.00	-1.0	60.2	7832
D	/D3107-GLY O A	/A0421-LYS C	3.83MM	-1	4.58	-1.0	-1.00	-1.0	34.8	7839
D	/D3107-GLY C A	/A0422-GLN N	3.76MM	-1	5.48	-1.0	-1.00	-1.0	115.7	7851
D	/D3107-GLY O A	/A0422-GLN N	2.84MM	-1	5.48	-1.0	-1.00	-1.0	106.7	7852
D	/D3107-GLY O A	/A0422-GLN CA	3.54MM	-1	5.48	-1.0	-1.00	-1.0	50.1	7856
D	/D3107-GLY O A	/A0422-GLN CB	3.75MS	-1	5.48	-1.0	-1.00	-1.0	70.5	7862
D	/D3109-TYR O A	/A0422-GLN CG	4.19MS	-1	6.08	-1.0	-1.00	-1.0	71.1	7867
D	/D3109-TYR N A	/A0422-GLN CD	3.89MS	-1	6.08	-1.0	-1.00	-1.0	154.5	7868
D	/D3109-TYR O A	/A0422-GLN CD	3.97MS	-1	6.08	-1.0	-1.00	-1.0	2.96	7869
D	/D3108-GLU CA A	/A0422-GLN OE1	3.65MS	-1	5.39	-1.0	-1.00	-1.0	123.6	7870
D	/D3108-GLU CG A	/A0422-GLN OE1	3.98SS	-1	5.39	-1.0	-1.00	-1.0	121.3	7871
D	/D3108-GLU C A	/A0422-GLN OE1	3.63MS	-1	5.39	-1.0	-1.00	-1.0	126.1	7872
D	/D3109-TYR N A	/A0422-GLN OE1	2.73MS	-1	6.08	-1.0	-1.00	-1.0	141.7	7873
D	/D3109-TYR CA A	/A0422-GLN OE1	3.75MS	-1	6.08	-1.0	-1.00	-1.0	159.9	7874
D	/D3109-TYR C A	/A0422-GLN OE1	3.34MS	-1	6.08	-1.0	-1.00	-1.0	157.4	7875
D	/D3109-TYR O A	/A0422-GLN OE1	3.13MS	-1	6.08	-1.0	-1.00	-1.0	147.2	7876
D	/D3110-ASP N A	/A0422-GLN OE1	4.12MS	-1	8.19	-1.0	-1.00	-1.0	125.8	7877
D	/D3107-GLY O A	/A0422-GLN C	3.68MM	-1	5.48	-1.0	-1.00	-1.0	50.6	7878
D	/D3107-GLY C A	/A0423-ILE N	3.93MM	-1	4.58	-1.0	-1.00	-1.0	4.68	7887
D	/D3107-GLY O A	/A0423-ILE N	2.89MM	-1	4.58	-1.0	-1.00	-1.0	157.4	7906
D	/D3107-GLY O A	/A0423-ILE CA	3.85MM	-1	4.58	-1.0	-1.00	-1.0	112.0	7907
D	/D3103-GLU OE2 A	/A0423-ILE CB	3.55SS	-1	8.19	-1.0	-1.00	-1.0	116.5	7911
D	/D3107-GLY CA A	/A0423-ILE CB	4.16MS	-1	4.58	-1.0	-1.00	-1.0	40.3	7915
D	/D3107-GLY O A	/A0423-ILE CB	3.77MS	-1	4.58	-1.0	-1.00	-1.0	72.3	7916
D	/D3103-GLU OE2 A	/A0423-ILE CG2	4.13SS	-1	8.19	-1.0	-1.00	-1.0	91.1	7917
D	/D3103-GLU OE2 A	/A0423-ILE CG1	3.42SS	-1	8.19	-1.0	-1.00	-1.0	70.4	7925
D	/D3107-GLY O A	/A0423-ILE CG1	3.56MS	-1	4.58	-1.0	-1.00	-1.0	57.2	7927
D	/D3109-TYR CB A	/A0423-ILE CG1	4.14SS	-1	7.14	-1.0	-1.00	-1.0	82.2	7928
D	/D3107-GLY CA A	/A0423-ILE O	3.80MM	-1	4.58	-1.0	-1.00	-1.0	85.6	7929
D	/D3107-GLY O A	/A0423-ILE O	4.15MM	-1	4.58	-1.0	-1.00	-1.0	82.8	7943
D	/D3109-TYR CD1 A	/A0434-MET SD	3.83SS	-1	8.37	-1.0	-1.00	-1.0	127.6	7944
D	/D3111-ASN ND2 A	/A0434-MET SD	3.36SS	-1	9.75	-1.0	-1.00	-1.0	96.5	8274
D	/D3052-ILE CD1 A	/A0434-MET CE	4.03SS	-1	9.75	-1.0	-1.00	-1.0	119.5	8275
D	/D3111-ASN ND2 A	/A0434-MET CE	2.94SS	-1	9.75	-1.0	-1.00	-1.0	121.6	8278
D	/D3110-ASP O A	/A0437-PRO CD	3.90MS	-1	6.08	-1.0	-1.00	-1.0	2.73	8279
D	/D3109-TYR O A	/A0437-PRO CG	3.99MS	-1	7.55	-1.0	-1.00	-1.0	74.8	8341
D	/D3110-ASP CA A	/A0437-PRO CG	3.96MS	-1	6.08	-1.0	-1.00	-1.0	58.9	8348



Page 2-A

**Declaration and Power of Attorney**

I hereby claim the benefit under Title 35, United States Code, Section 119(e) of any United States provisional application(s) listed below:

<u>Provisional Application No.</u>	<u>Filing Date</u>	<u>Signer</u>
_____	_____	_____
_____	_____	_____
_____	_____	_____
_____	_____	_____
_____	_____	_____

I hereby claim the benefit under Title 35, United States Code, Section 120 of any United States Application(s), or Section 363(c) of any PCT International Application(s) designating the United States listed below. Insofar as this application discloses and claims subject matter in addition to that disclosed in any such prior Application in the manner provided by the first paragraph of Title 35, United States Code, Section 112, I acknowledge the duty to disclose to the United States Patent and Trademark Office all information known to me to be material to patentability as defined in Title 37, Code of Federal Regulations, Section 1.56, which became available between the filing date(s) of such prior Application(s) and the national or PCT international filing date of this application:

<u>Application Serial No.</u>	<u>Filing Date</u>	<u>Signer</u>
<u>08/966,987</u>	<u>November 10, 1997</u>	_____
<u>08/967,403</u>	<u>November 10, 1997</u>	_____
<u>08/966,932</u>	<u>November 10, 1997</u>	_____
<u>08/967,148</u>	<u>November 10, 1997</u>	_____
_____	_____	_____
_____	_____	_____

**And I hereby appoint**

John P. White (Reg. No. 28,678); Christopher C. Dunham (Reg. No. 22,031); Norman H. Zivin (Reg. No. 25,385); Jay H. Maioli (Reg. No. 27,213); William E. Pelton (Reg. No. 25,702); Robert D. Katz (Reg. No. 30,141); Peter J. Phillips (Reg. No. 29,691); Wendy E. Miller (Reg. No. 35,615); Richard S. Milner (Reg. No. 33,970); Robert T. Maldonado (Reg. No. 38,232); Paul Teng (Reg. No. 40,837); Richard F. Jaworski (Reg. No. 33,515); Alan J. Morrison (Reg. No. 37,399); Mark A. Farley (Reg. No. 33,170); Pedro C. Fernandez (Reg. No. 41,741); Gary J. Gershik (Reg. No. 39,992); Alan D. Miller (Reg. No. 42,889); Frank Bruno (Reg. No. 46,583); and Christine S. Nickles (Reg. No. 51,103)

and each of them, all c/o Cooper & Dunham LLP, 1185 Avenue of the Americas, New York, New York 10036, my attorneys, each with full power of substitution and revocation, to prosecute this application, to make alterations and amendments therein, to receive the patent, to transact all business in the Patent and Trademark Office connected therewith and to file any International Applications which are based thereon under the provisions of the Patent Cooperation Treaty.

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**Declaration and Power of Attorney**

I hereby claim the benefit under Title 35, United States Code, Section 119(e) of any United States provisional application(s) listed below:

<u>Provisional Application No.</u>	<u>Filing Date</u>	<u>Signer</u>
_____	_____	_____
_____	_____	_____
_____	_____	_____
_____	_____	_____
_____	_____	_____

I hereby claim the benefit under Title 35, United States Code, Section 120 of any United States Application(s), or Section 365(c) of any PCT International Application(s) designating the United States listed below. Insofar as this application discloses and claims subject matter in addition to that disclosed in any such prior Application in the manner provided by the first paragraph of Title 35, United States Code, Section 112, I acknowledge the duty to disclose to the United States Patent and Trademark Office all information known to me to be material to patentability as defined in Title 37, Code of Federal Regulations, Section 1.56, which become available between the filing date(s) of such prior Application(s) and the national or PCT international filing date of this application:

<u>Application Serial No.</u>	<u>Filing Date</u>	<u>Signer</u>
09/100,631	June 18, 1998	_____
09/100,763	June 18, 1998	_____
09/100,529	June 18, 1998	_____
09/100,762	June 18, 1998	_____
09/100,521	June 18, 1998	_____
08/976,741	November 24, 1997	_____

**And I hereby appoint**

19- John P. White (Reg. No. 28,678); Christopher C. Dunham (Reg. No. 22,031); Norman H. Zivin (Reg. No. 25,385); Jay H. Maioli (Reg. No. 27,213); William E. Pelton (Reg. No. 25,702); Robert D. Katz (Reg. No. 30,141); Peter J. Phillips (Reg. No. 29,691); Wendy E. Miller (Reg. No. 35,615); Richard S. Milner (Reg. No. 33,970); Robert T. Maldonado (Reg. No. 38,232); Paul Teng (Reg. No. 40,837); Richard F. Jaworski (Reg. No. 33,515); Alan J. Morrison (Reg. No. 37,399); Mark A. Farley (Reg. No. 33,170); Pedro C. Fernandez (Reg. No. 41,741); Gary J. Gershik (Reg. No. 39,992); Alan D. Miller (Reg. No. 42,889); Frank Bruno (Reg. No. 46,583); and Christine S. Nickles (Reg. No. 51,103)

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## Declaration and Power of Attorney

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

Full name of sole or  
first joint inventor Richard T. Wyatt

Inventor's signature Richard T. Wyatt

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Citizenship \_\_\_\_\_ Date of signature \_\_\_\_\_

Residence \_\_\_\_\_

Post Office Address \_\_\_\_\_

Full name of joint  
inventor (if any) \_\_\_\_\_

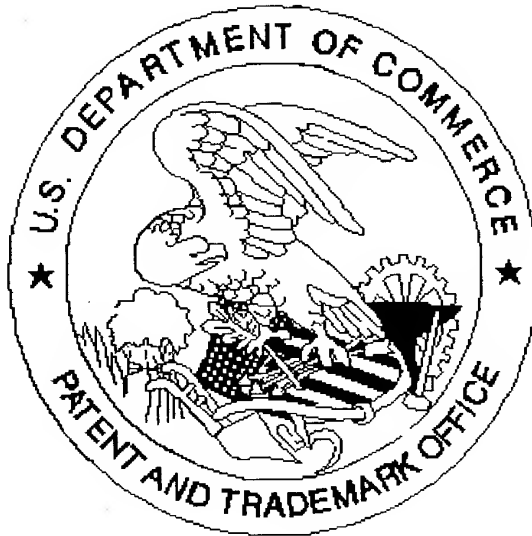
Inventor's signature \_\_\_\_\_

Citizenship \_\_\_\_\_ Date of signature \_\_\_\_\_

Residence \_\_\_\_\_

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